optimization

November 29, 2022

1 Write a script that implement the GD algorithm, with the following structure:

Input: f: the function f(x) we want to optimize. It is supposed to be a Python function, not an array. grad_f: the gradient of f(x). It is supposed to be a Python function, not an array. x0: an n-dimensional array which represents the initial iterate. kmax: an integer. The maximum possible number of iterations (to avoid infinite loops) tolf: small float. The relative tollerance of the algorithm. Convergence happens if $||grad_f(x_k)||^2 < tolf ||grad_f(x_0)||^2$ tolx: small float. The tollerance in the input domain. Convergence happens if $||x_k|^2 - x_k^2|^2 = (1 + 1) = (1$

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

```
[72]: def plot(x, errf, x_true=False, back=False, alpha=0.2):
          k = len(x)
          title = f"{'x*= ' + str(x_true) if x_true else ''} x_c={np.round(x[-1],_
        الله على ال
        →+ str(alpha) if not back else ''}"
          plt.title(title)
          plt.plot(errf)
          legend = ["error"]
          if x true:
               x errors = np.zeros(x.shape)
               for i, x_k in enumerate(x):
                   x errors[i] = np.linalg.norm(x k - x true)
               plt.plot(x_errors)
               legend.append("X error")
           #plt.subplot(2, 2, 2)
           #plt.plot(points, grads)
           #plt.subplot(2, 2, 3)
           #plt.plot(points, err)
```

```
plt.legend(legend)
    plt.show()
def backtracking(f, grad_f, x):
    This function is a simple implementation of the backtracking algorithm for
    the GD (Gradient Descent) method.
    f: function. The function that we want to optimize.
    grad_f: function. The gradient of f(x).
    x: ndarray. The actual iterate x_k.
    alpha = 1
    c = 0.8
    tau = 0.25
    while f(x - alpha * grad_f(x)) > f(x) - c * alpha * np.linalg.
 \rightarrownorm(grad_f(x), 2) ** 2:
        alpha = tau * alpha
        if alpha < 1e-3:
            break
    return alpha
def GD(f, grad_f, x0, tolf, tolx, kmax, alpha=0.2, back=False):
    x0 = np.array(x0)
    shape = (kmax, *x0.shape)
    # output
    x = np.zeros(shape)
    f_val = np.zeros(shape)
    grads = np.zeros(shape)
    err = np.zeros(shape)
   x_{tol} = tolx
   f_tol = tolf
   x_old = x0
    k = 0
    while k < kmax and x_tol >= tolx and f_tol >= tolf:
        if back:
            alpha = backtracking(f, grad_f, x_old)
        x_k = x_old - alpha * np.array(grad_f(x_old))
        x_tol = np.linalg.norm(x_k-x_old)
```

```
f_tol = np.linalg.norm(f(x_k))

# Update arrays
x[k] = x_k
f_val[k] = f(x_k)
grads[k] = grad_f(x_k)
err[k] = np.linalg.norm(grads[k])
x_old = x_k
k = k+1

return x[:k], f_val[:k], grads[:k], err[:k]
```

1.1 Test the algorithm above on the following functions:

```
[73]: tolf = 1e-4
tolx = 1e-4
kmax = 100
alphas = [0.1, 0.01]
```

1.1.1 Function 1

$$f(x_1,x_2) = (x_1-3)^2 + (x_2-1)^2 \\$$

for which the true optimum is $x^* = (3,1)^T$

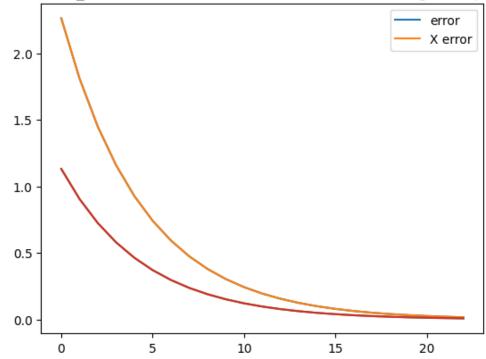
```
[74]: def f1(x):
          x1, x2 = x
          return (x1 - 3)**2 + (x2 - 1)**2
      def grad_f1(x):
          x1, x2 = x
          return np.array((2*(x1-3), 2*(x2-1)))
      x0 = (2, 2)
      x_{true1} = (3, 1)
      def test_function(f, grad_f, x0, kmax, x_true=False, f5=False):
          for alpha in alphas:
              x, f_val, grads, err = GD(f, grad_f, x0, tolf, tolx, kmax, alpha)
              plot(x, err, x_true, alpha=alpha)
              if f5:
                  x_ = np.linspace(-3, 3, 1000)
                  plt.plot(x_, f(x_))
                  plt.plot(x, f_val, "bo")
```

```
plt.show()
x, f_val, grads, err = GD(f, grad_f, x0, tolf, tolx, kmax, back=True)
plot(x, err, x_true)

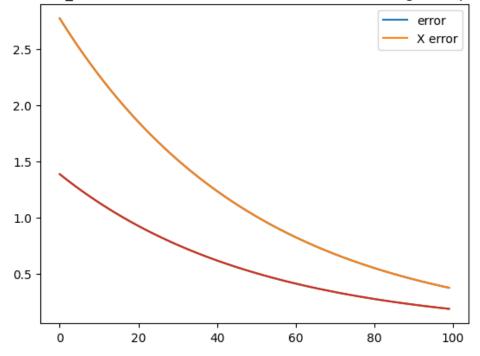
if f5:
    x_ = np.linspace(-3, 3, 1000)
    plt.plot(x_, f(x_))
    plt.plot(x, f_val, "bo")
    plt.show()

test_function(f1, grad_f1, x0, kmax, x_true1)
```

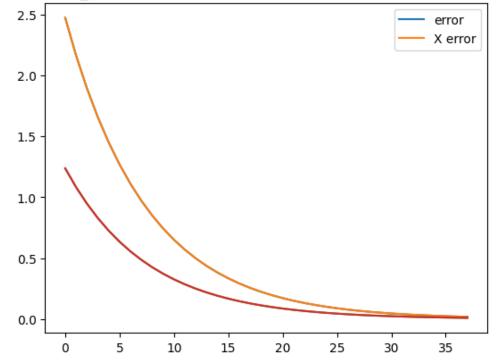
 $x^*=(3, 1) x_c=[2.99 \ 1.01] \ N.$ of iteration: 23, backtracking: no alpha: 0.1



 $x^*=$ (3, 1) $x_c=[2.87 \ 1.13]$ N. of iteration: 100, backtracking: no alpha: 0.01



 $x^* = (3, 1) x_c = [2.99 \ 1.01] N.$ of iteration: 38, backtracking: no alpha: 0.2



1.2 Function 2

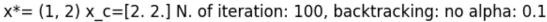
$$f(x_1, x_2) = 10(x_1 - 1)^2 + (x_2 - 2)^2$$

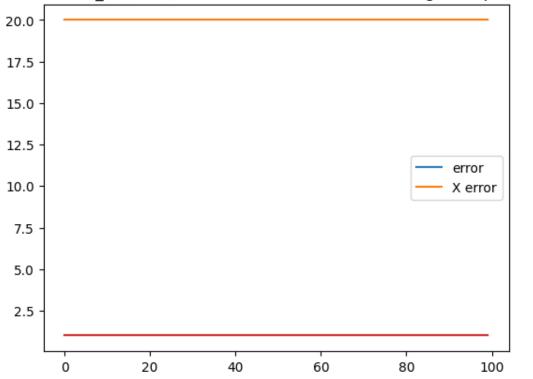
```
[75]: def f2(x):
    x1, x2 = x
    return 10*(x1 - 1)**2 + (x2 - 2)**2

def grad_f2(x):
    x1, x2 = x
    return np.array((20*(x1-1), 2*(x2-2)))

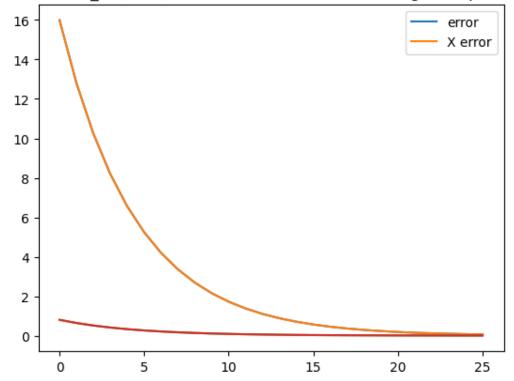
x0 = (2, 2)
x_true2 = (1,2)

test_function(f2, grad_f2, x0, kmax, x_true2)
```

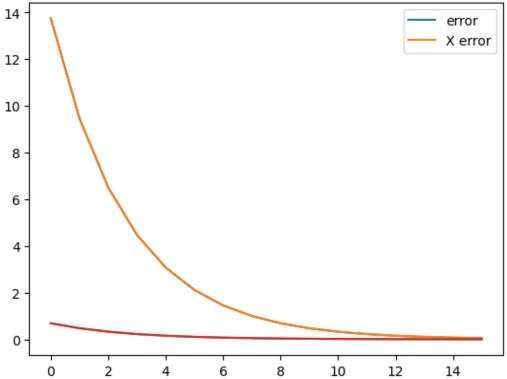




 $x^*=(1, 2) x_c=[1, 2] N.$ of iteration: 26, backtracking: no alpha: 0.01







1.3 Function 3

$$f(x) = \frac{1}{2}||Ax - b||_2^2$$

```
[76]: def f3(x):
    x = np.array(x)
    x = np.reshape(x,(1, len(x)))
    n, m = x.shape
    x_true = np.ones((1, n))
    v = np.linspace(0, 1, n, endpoint=True)
    A = numpy.vander(v)
    b = A @ x_true
    return 1/2 * np.linalg.norm(A @ x - b, 2)**2

def grad_f3(x):
    n = len(x)
    v = np.linspace(0,1,n)
    A = np.vander(v)
    x_true = np.ones(n).T
    b = A @ x_true
```

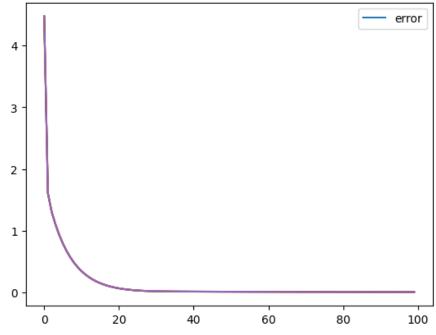
```
return np.array(A.T@(A@x-b))

N = [5, 10, 15]

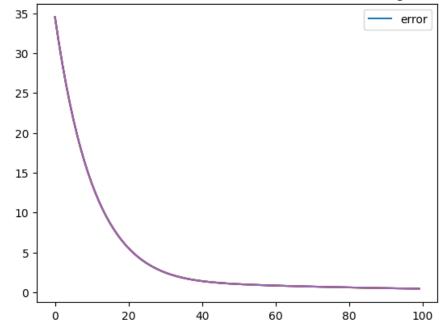
for n in N:
    x0 = [3 for i in range(n)]
    print("N = ", n)
    test_function(f3, grad_f3, x0, kmax)
```

N = 5

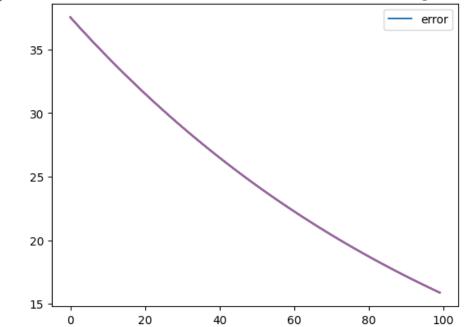
x_c=[1.06 1.02 0.98 0.95 1.02] N. of iteration: 100, backtracking: no alpha: 0.1



x_c=[1.25 1.17 1.07 0.91 0.83] N. of iteration: 100, backtracking: no alpha: 0.01

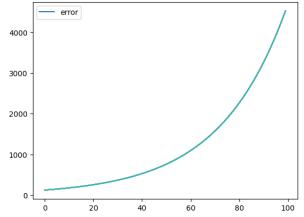


x_c=[2.18 2.12 2.03 1.87 1.43] N. of iteration: 100, backtracking: no alpha: 0.2

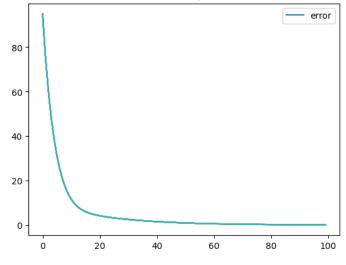


N = 10

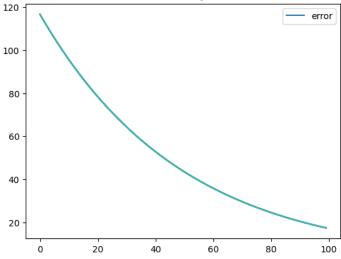
x_c=[42.68 44.36 46.44 49.07 52.47 57.04 63.5 73.38 90.72 136.79] N. of iteration: 100, backtracking: no alpha: 0.1



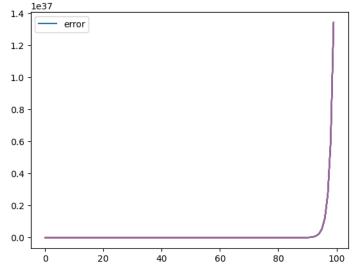
 $x_c = [1.17 \ 1.14 \ 1.1 \ 1.06 \ 1.01 \ 0.96 \ 0.9 \ 0.85 \ 0.85 \ 1.09]$ N. of iteration: 100, backtracking: no alpha: 0.01



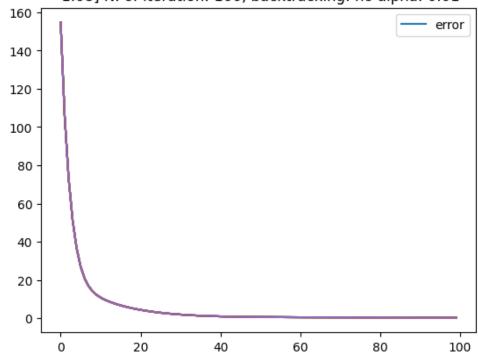
x_c=[1.81 1.77 1.72 1.67 1.6 1.52 1.4 1.25 1.01 0.54] N. of iteration: 100, backtracking: no alpha: 0.2



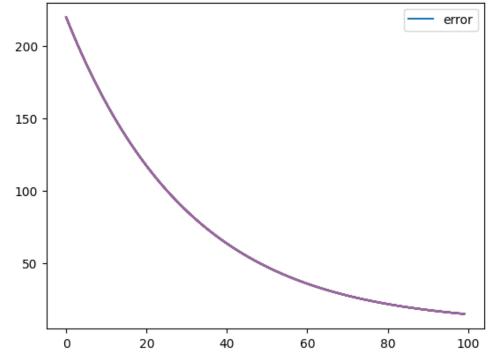
N = 15



x_c=[1.14 1.13 1.1 1.08 1.06 1.03 1.01 0.98 0.95 0.92 0.9 0.89 0.9 0.95 1.08] N. of iteration: 100, backtracking: no alpha: 0.01



 $x_c = [1.63\ 1.6\ 1.57\ 1.54\ 1.5\ 1.46\ 1.41\ 1.36\ 1.29\ 1.21\ 1.12\ 1.$ 0.86 0.67 0.42] N. of iteration: 100, backtracking: no alpha: 0.2



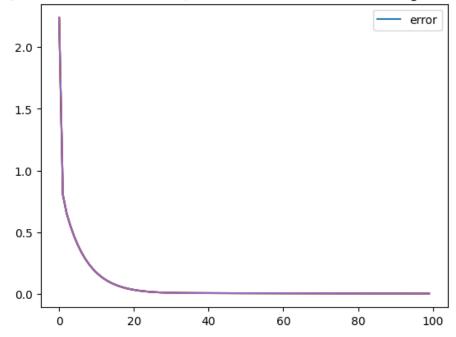
1.4 Function 4

$$f(x) = \frac{1}{2}||Ax - b||_2^2 + \frac{\lambda}{2}||x||_2^2$$

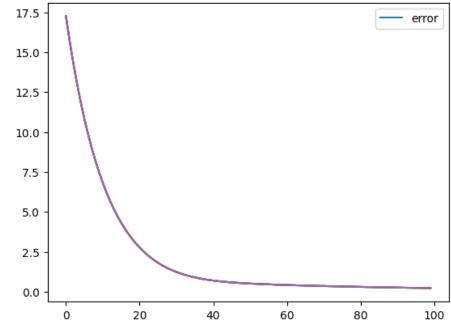
```
[77]: def f4_builder(lmb):
          def f4(x):
              x = np.array(x)
              x = np.reshape(x, (1, len(x)))
              n, m = x.shape
              x_{true} = np.ones((1, n))
              v = np.linspace(0, 1, n, endpoint=True)
              A = numpy.vander(v)
              b = A @ x_true
              return 1/2 * np.linalg.norm(A @ x - b, 2)**2 + lmb/2 * np.linalg.
       \rightarrownorm(x)**2
          return f4
      def grad_f4_builder(lmb):
          def grad_f4(x):
              n = len(x)
              v = np.linspace(0,1,n)
              A = np.vander(v)
              x_true = np.ones(n).T
              b = A @ x_true
              return np.array(A.T@(A@x-b)) + lmb*x
          return grad_f4
      n = 5
      lmbs = np.linspace(0, 1, 3)
      x0 = [0 \text{ for i in } range(n)]
      for lmb in lmbs:
          print("Lambda: ", lmb)
          f4 = f4_builder(lmb)
          grad_f4 = grad_f4_builder(lmb)
          test_function(f4, grad_f4, x0, kmax)
```

Lambda: 0.0

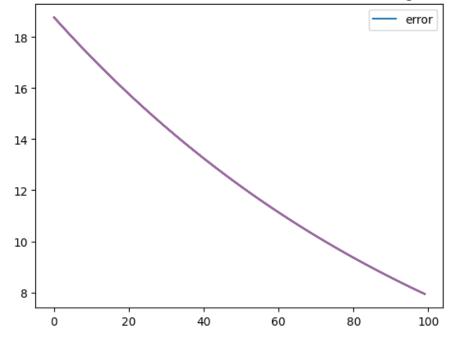
x_c=[0.97 0.99 1.01 1.03 0.99] N. of iteration: 100, backtracking: no alpha: 0.1



x_c=[0.87 0.91 0.97 1.04 1.08] N. of iteration: 100, backtracking: no alpha: 0.01

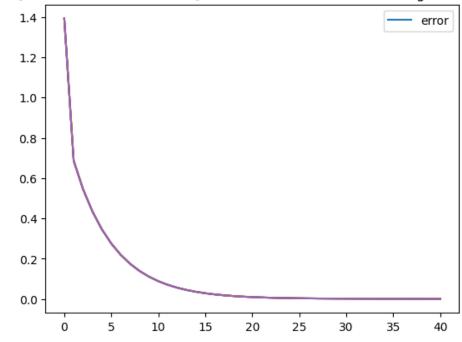


x_c=[0.41 0.44 0.49 0.57 0.79] N. of iteration: 100, backtracking: no alpha: 0.2

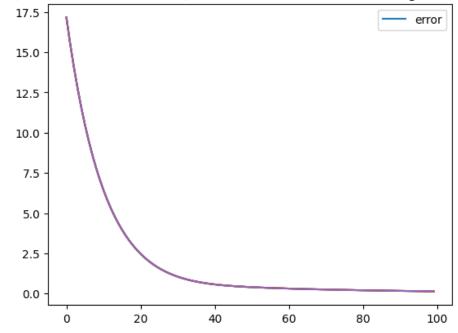


Lambda: 0.5

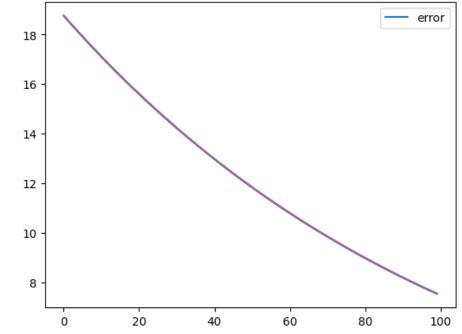
x_c=[0.84 0.87 0.92 0.98 1.02] N. of iteration: 41, backtracking: no alpha: 0.1



x_c=[0.8 0.84 0.89 0.98 1.07] N. of iteration: 100, backtracking: no alpha: 0.01

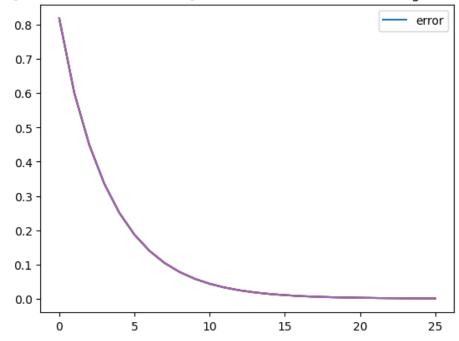


 $x_c=[0.4\ 0.43\ 0.48\ 0.56\ 0.77]$ N. of iteration: 100, backtracking: no alpha: 0.2

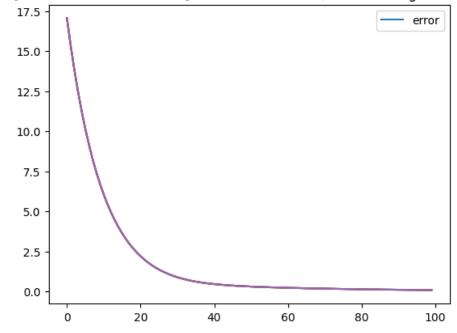


Lambda: 1.0

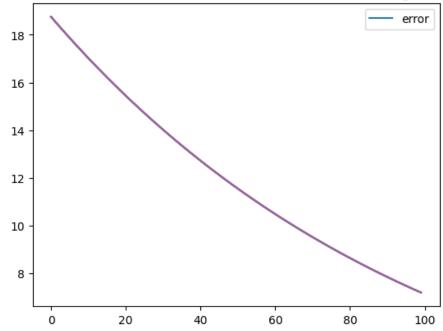
 $x_c=[0.76\ 0.79\ 0.84\ 0.92\ 1.02]$ N. of iteration: 26, backtracking: no alpha: 0.1



x_c=[0.74 0.78 0.83 0.92 1.05] N. of iteration: 100, backtracking: no alpha: 0.01







1.4.1 Function 5

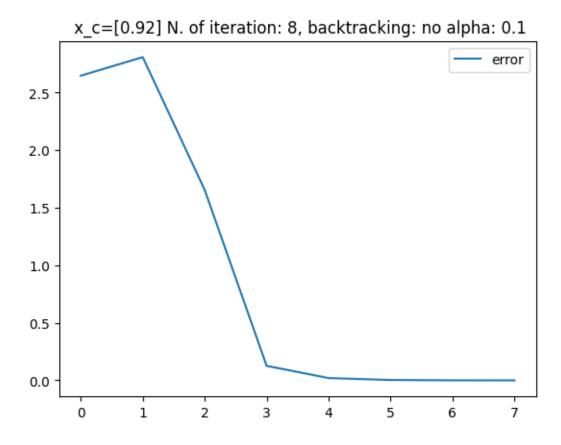
$$f(x) = x^4 + x^3 - 2x^2 - 2x$$

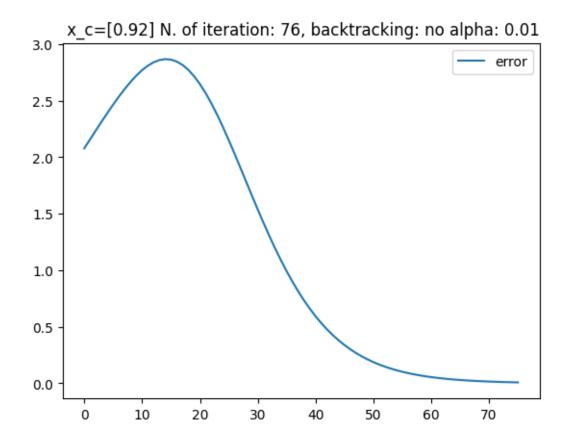
```
[78]: def f5(x):
    return np.power(x,4) + np.power(x, 3) - 2*np.power(x,2) - 2*x

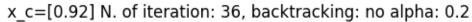
def grad_f5(x):
    return np.array(4*np.power(x, 3) + 3*np.power(x,2) - 4*x - 2)

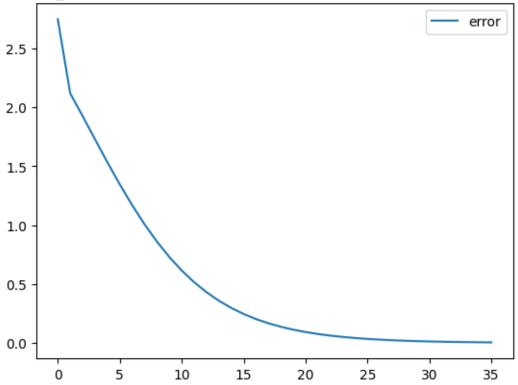
N = np.arange(5, 20, 5)

x0 = [0.]
test_function(f5, grad_f5, x0, kmax)
```







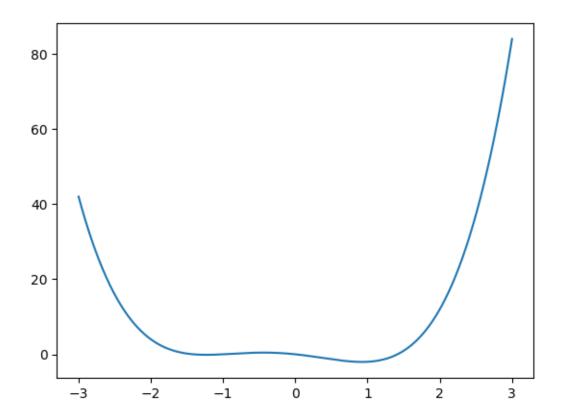


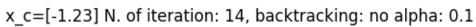
Only for the non-convex function defined in 5, plot it in the interval [-3, 3] and test the convergence point of GD with different values of x0 and different step-sizes. Observe when the convergence point is the global minimum and when it stops on a local minimum or maximum.

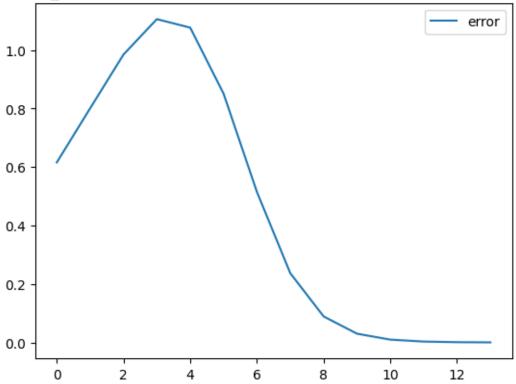
```
[79]: x_5 = np.linspace(-3, 3, 1000)
plt.plot(x_5, f5(x_5))
plt.show()

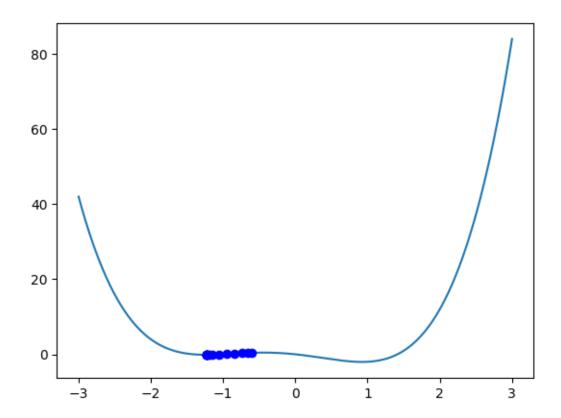
starting_points = [-2, 0, 2]

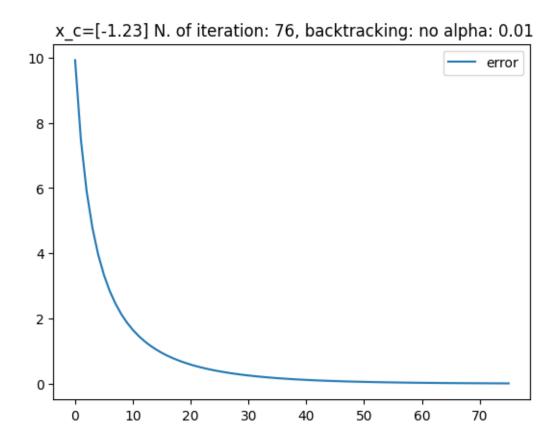
for x0 in starting_points:
    x0 = np.array([x0])
    test_function(f5, grad_f5, x0, kmax, f5=True)
```

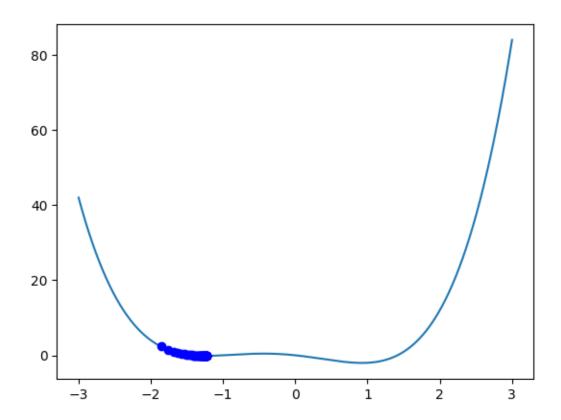




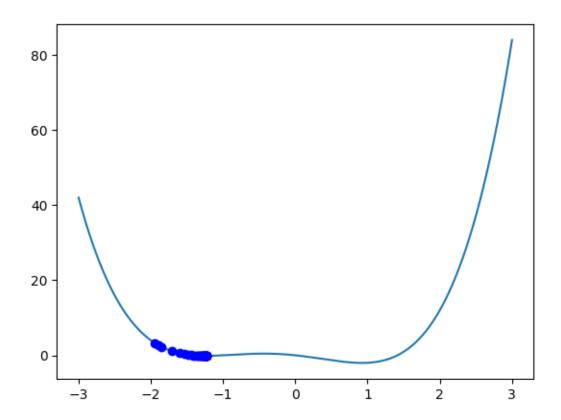




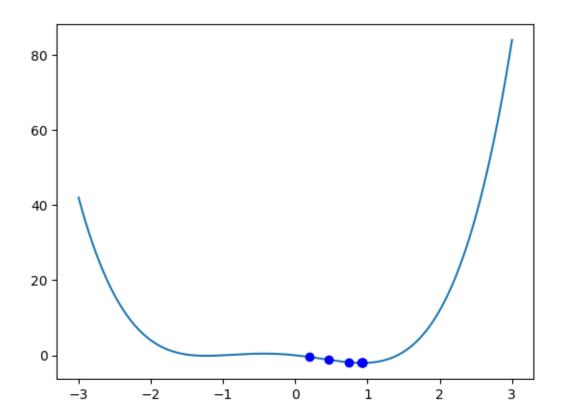


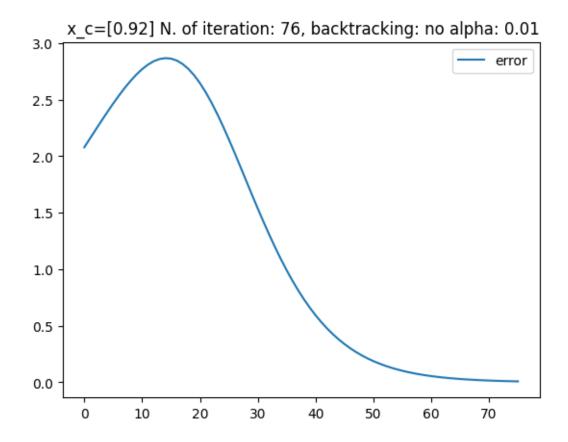


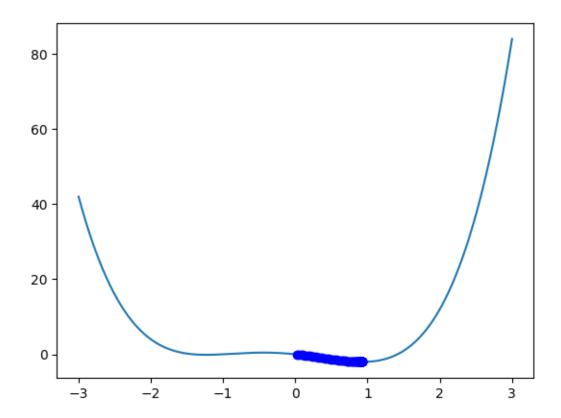
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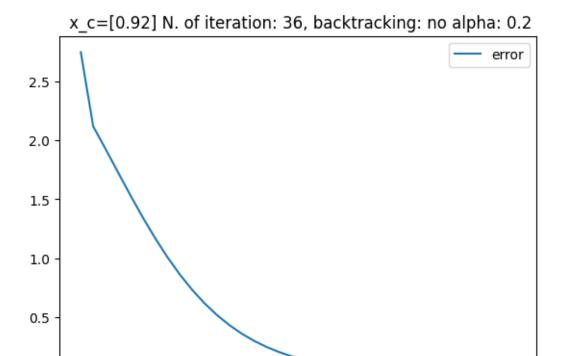


 $x_c=[0.92]$ N. of iteration: 8, backtracking: no alpha: 0.1 error 2.5 2.0 1.5 1.0 0.5 0.0 2 3 4 5 6 ò i 7



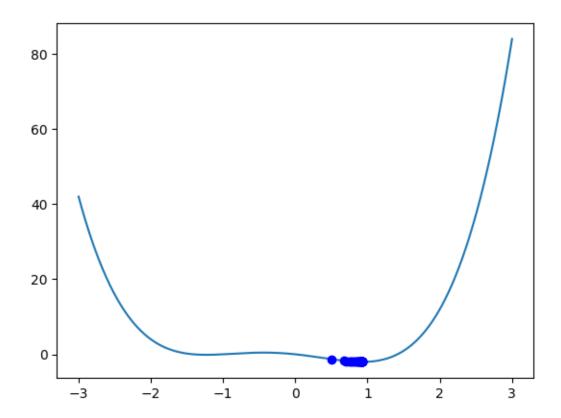


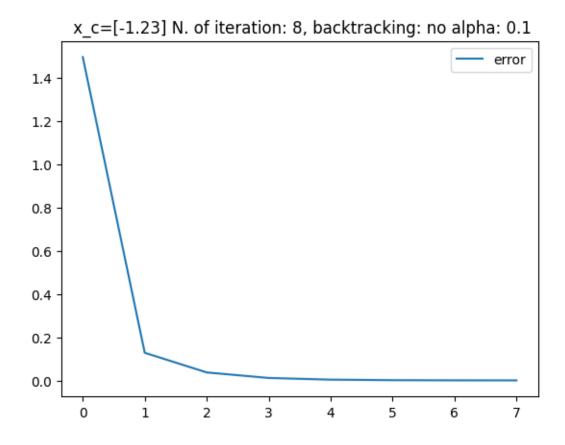


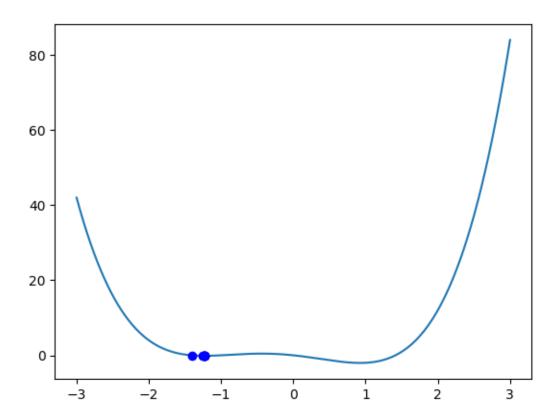


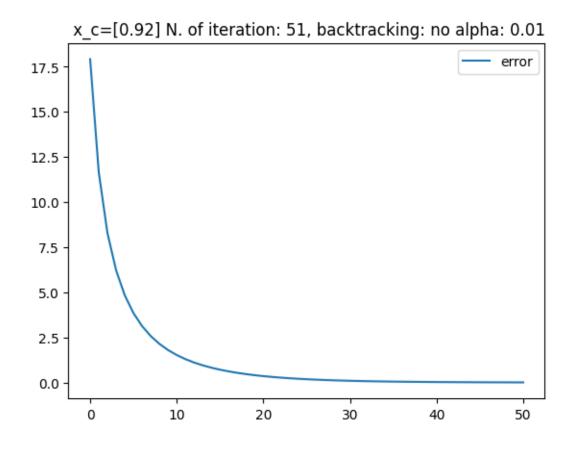
0.0

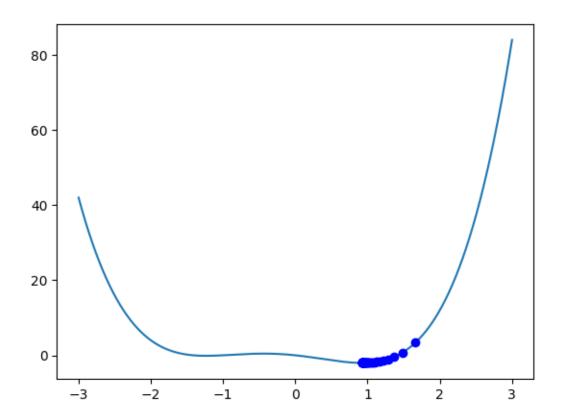
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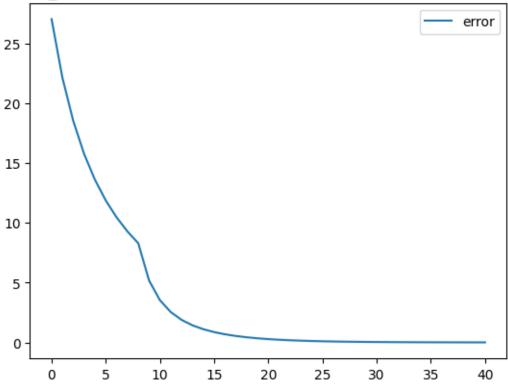


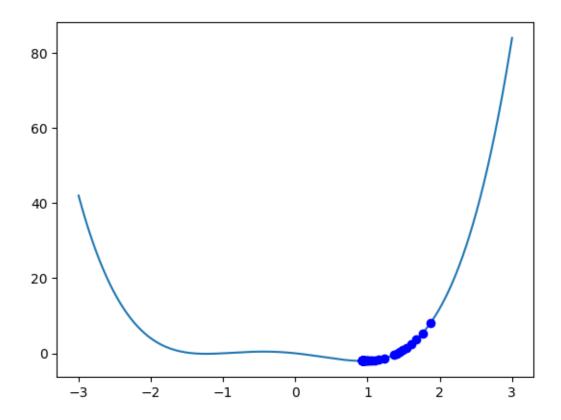






 $x_c=[0.92]$ N. of iteration: 41, backtracking: no alpha: 0.2





Hard (optional): For the functions 1 and 2, plot the contour around the minimum and the path defined by the iterations (following the example seen during the lesson). See plt.contour to do that.

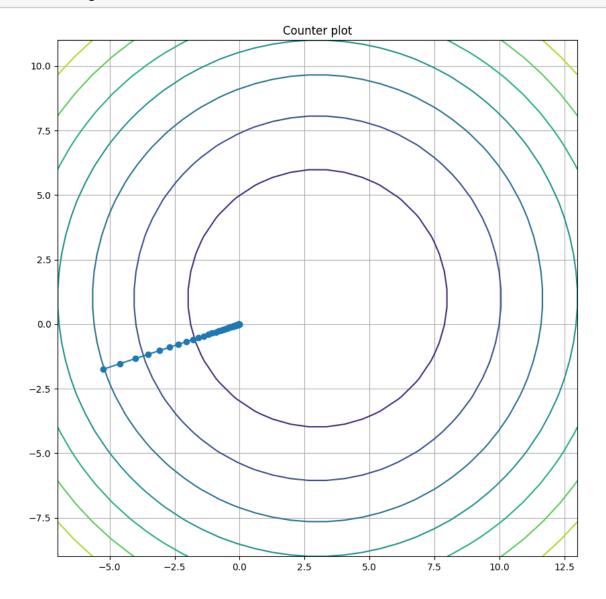
```
[80]: def contour(f, grad_f, x0, x_true, radius, tolx, tolf, kmax):
    x11, x12 = x_true

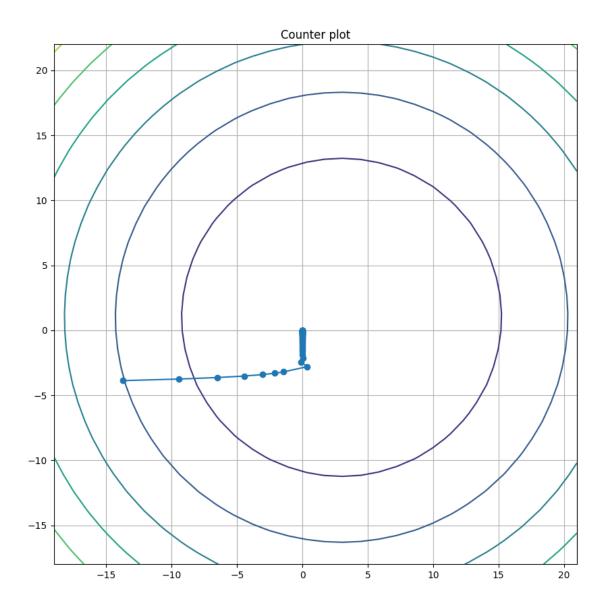
    xv = np.linspace(x11 - radius, x11 + radius, 30)
    yv = np.linspace(x12 - radius, x12 + radius, 30)
    xx, yy = np.meshgrid(xv, yv)

    x, f_val, grads, err = GD(f, grad_f, x0, tolf, tolx, kmax, back=True)
    zz = f1((xx, yy))

    plt.figure(figsize=(10,10))
    plt.contour(xx, yy, zz)
    plt.plot(grads[:, 0], grads[:, 1], 'o-')
    plt.title("Counter plot")
    plt.grid()
    plt.show()

contour(f1, grad_f1, (0, 0), x_true1, 10, tolx, tolf, kmax)
```





2 Optimization via Stochastic Gradient DescentInput:

l: the function l(w; D) we want to optimize. It is supposed to be a Python function, not an array. grad_l: the gradient of l(w; D). It is supposed to be a Python function, not an array. w0: an n-dimensional array which represents the initial iterate. By default, it should be randomly sampled. data: a tuple (x, y) that contains the two arrays x and y, where x is the input data, y is the output data. batch_size: an integer. The dimension of each batch. Should be a divisor of the number of data. n_epochs: an integer. The number of epochs you want to reapeat the iterations. Output: w: an array that contains the value of w_k FOR EACH iterate w_k (not only the latter). f_val: an array that contains the value of $l(w_k; D)$ FOR EACH iterate w_k ONLY after each epoch. grads: an array that contains the value of $grad_l(w_k; D)$ FOR EACH iterate w_k ONLY after each epoch. err: an array the contains the value of $|grad_l(w_k; D)|_2$ FOR EACH iterate w_k

ONLY after each epoch.

#Y1 = Y[I1] #Y2 = Y[I2]

```
[81]: # Import the data MNIST
      import numpy as np
      import pandas as pd
      import matplotlib.pyplot as plt
      import scipy as sp
      dataset = pd.read_csv("data.csv")
      dataset = np.array(dataset)
      def split(X, Y, Ntrain):
          d, N = X.shape
          idx = np.arange(N)
          np.random.shuffle(idx)
          train_idx = idx[:Ntrain]
          test_idx = idx[Ntrain:]
          Xtrain = X[:, train_idx]
          Ytrain = Y[train_idx]
          Xtest = X[:, test_idx]
          Ytest = Y[test_idx]
          return (Xtrain, Xtest, Ytrain, Ytest)
[82]: def create_dataset(dataset, digits=[3,6], Ntrain=4600):
          digits = [3, 6]
          y = dataset[:, 0]
          x = dataset[:, 1:].T
          Y = y # y.reshape((len(y), 1))
          X = np.concatenate((np.ones((1, len(y))), x), axis=0)
          I1 = (Y == digits[0]) # (Y[:, 0] == digits[0])
          I2 = (Y == digits[1]) # (Y[:, 0] == digits[1])
          X1 = X[:, I1]
          X2 = X[:, I2]
          Y1 = np.zeros((len(Y[I1]), ))
          Y2 = np.ones((len(Y[I2]), ))
```

```
X = np.concatenate((X1, X2), axis=1)
          Y = np.concatenate((Y1, Y2))
          d, N = X.shape
          #Ntrain = 4600#int(N/3*2)
          x_train, x_test, y_train, y_test = split(X, Y, Ntrain)
          return x_train, x_test, y_train, y_test
[83]: x_train, x_test, y_train, y_test = create_dataset(dataset)
      print(x_train.shape, x_test.shape, y_train.shape)
     (785, 4600) (785, 3888) (4600,)
[84]: def sigmoid(x):
          return 1 / (1 + np.exp(-x))
      def f(x, w):
         x_cup = x
          return sigmoid(x_cup.T @ w)
      def grad_f(x):
          return np.exp(-x) / (np.exp(-x) + 1) ** 2
      def 1(w, x, y):
          return np.mean(np.linalg.norm(f(x, w)-y)**2)
      def loss_grad(w, x, y):
         d, n = x.shape
          y = np.array(y)
          sum = 0
          for i in range(n):
              z = f(x[:, i], w)
              sum += z * (1 - z) * x[:, i].T * (z - y[i])
          return sum / n
      def grad_1(w, x, y):
```

 $x_cup = x$

```
\hookrightarrow (f(x, w) - y))
[85]: n epochs = 50
[86]: batch_size = 15
      def batch(x, y, batch_size):
          n = x.shape[1]
          idx = np.arange(n)
          np.random.shuffle(idx)
          n_batches = n // batch_size
          for i in range(n_batches):
              batch_index = idx[i*batch_size:(i+1)*batch_size]
              yield x[:, batch_index], y[batch_index]
      def SGD(1, grad_1, w0, data, batch_size, n_epochs=50):
          shape = (n_epochs, *w0.shape)
          x_, y_ = data
          d, n = x_.shape
          w = np.zeros(shape)
          f_val = np.zeros((n_epochs, 1))
          grads = np.zeros((n_epochs, 1, w0.shape[0]))
          err = np.zeros((n_epochs, 1))
          #print("WO shape: ", wO.shape)
          alpha = 1e-2
          w \text{ old} = w0
          w_k = w_old
          for epoch in range(n_epochs):
              batch_iterator = batch(x_, y_, batch_size)
              for x, y in batch_iterator:
                  grad = grad_l(w_old, x, y)
                  w_k = w_old - alpha * grad
                  w_old = w_k
              w[epoch] = w_k
              f_{val}[epoch] = l(w_k, x_, y_)
              grads[epoch] = grad_l(w_k, x_, y_)
              err[epoch] = np.linalg.norm(grads[epoch], 2)
          return w, f_val, grads, err
      data = (x_train, y_train)
```

return np.mean(sigmoid(x_cup.T @ w)*(1-sigmoid(x_cup.T @ w)) * x_cup.T *_u

```
sigma = 1e-3
d, N = x_train.shape
w0 = np.random.normal(0, sigma, (d, ))
w_sgd, f_val__sgd, grads_sgd, err_sgd = SGD(
    l, loss_grad, w0, data, batch_size, n_epochs)
```

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))

```
[87]: def predict(w, X, treshold=0.5):
    y_pred = f(X, w)
    y_copy = np.copy(y_pred)
    y_pred[y_copy < treshold] = 0
    y_pred[y_copy >= treshold] = 1
    return y_pred

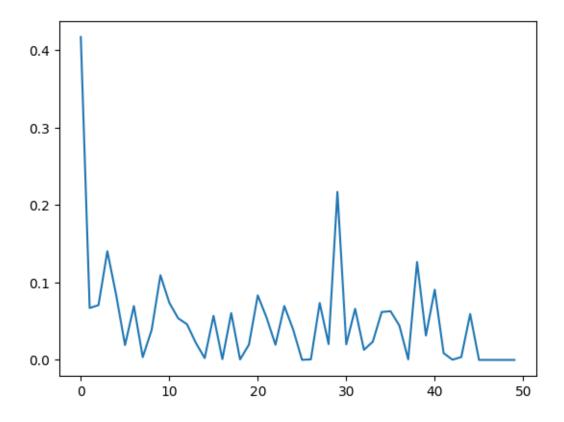
def accuracy(y_hat, y):
    return round(np.mean(y_hat == y), 10)
```

```
[88]: w_star_sgd = w_sgd[-1]
y_hat = predict(w_star_sgd, x_train)
print("Accuracy: ", accuracy(y_hat, y_train))
x_plot = np.arange(n_epochs)
plt.plot(x_plot, err_sgd)
plt.show()
```

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))

Accuracy: 0.9936956522



```
[89]: def GD2(f, grad_f, D, w0, tolf=1e-9, tolx=1e-9, kmax=50, alpha=0.1, back=False):
          x_{cup}, y = D
          shape = (kmax, *w0.shape)
          w = np.zeros(shape)
          f_val = np.zeros((kmax, 1))
          grads = np.zeros((kmax, 1, w0.shape[0]))
          err = np.zeros((kmax, 1))
          # output
          \#x\_cup = np.concatenate((np.ones((1, N)), X), axis=0)
          x_tol = tolx
          f_tol = tolf
          w_old = w0
          k = 0
          while k < kmax and x_tol >= tolx and f_tol >= tolf:
              if back:
                  alpha = backtracking(f, grad_f, w_old)
```

```
w_k = w_old - alpha * grad_f(w_old, x_cup, y)
x_tol = np.linalg.norm(w_k-w_old)
f_tol = np.linalg.norm(f(w_k, x_cup, y))

# Update arrays
w[k] = w_k
f_val[k] = f(w_k, x_cup, y)
grads[k] = grad_f(w_k, x_cup, y)
err[k] = np.linalg.norm(grads[k])
w_old = w_k
k = k+1

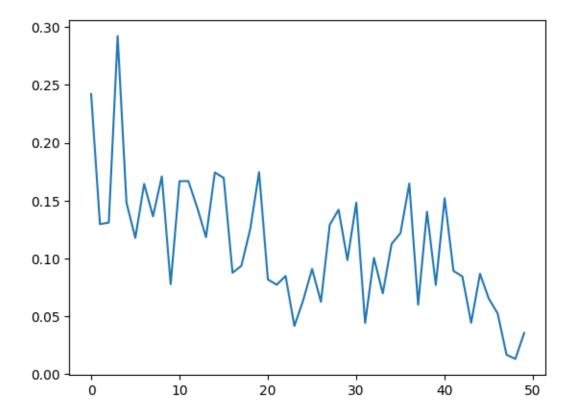
return w[:k], f_val[:k], grads[:k], err[:k]
```

```
[97]: sigma = 1e-3
w0 = np.random.normal(0, sigma, (d, ))
w_gd, f_val_gd, grads_gd, err_gd = GD2(1, loss_grad, (x_train, y_train), w0)
```

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))

```
[98]: w_star_gd = w_gd[-1]
x_plot = np.arange(len(w_gd))
plt.plot(x_plot, err_gd)
plt.show()
y_hat = predict(w_star_gd, x_train)
print("Accuracy: ", accuracy(y_hat, y_train))
```



Accuracy: 0.9531102733

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))

```
[92]: x_train, x_test, y_train, y_test = create_dataset(dataset, digits=[1, 7], U_ →Ntrain=dataset.shape[0]//2)
```

```
[103]: data = (x_train, y_train)
    sigma = 1e-3
    d, N = x_train.shape
    w0 = np.random.normal(0, sigma, (d, ))
    w_sgd, f_val_sgd, grads_sgd, err_sgd = SGD(
        l, loss_grad, w0, data, batch_size, n_epochs)

sigma = 1e-3
    w0 = np.random.normal(0, sigma, (d, ))
    w_gd, f_val_gd, grads_gd, err_gd = GD2(1, loss_grad, (x_train, y_train), w0)
```

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

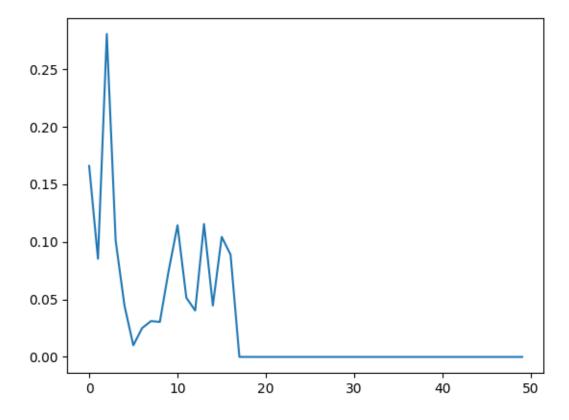
return 1 / (1 + np.exp(-x))

```
[104]: w_star_sgd = w_sgd[-1]
    y_hat = predict(w_star_sgd, x_train)
    print("Accuracy: ", accuracy(y_hat, y_train))
    x_plot = np.arange(n_epochs)
    plt.plot(x_plot, err_sgd)
    plt.show()
```

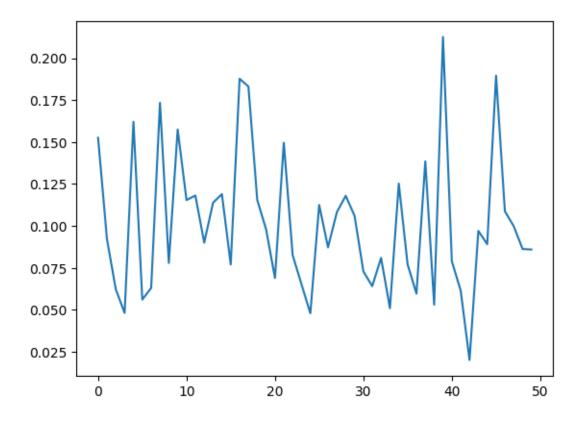
/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))

Accuracy: 0.9917530631



```
[105]: w_star_gd = w_gd[-1]
    x_plot = np.arange(len(w_gd))
    plt.plot(x_plot, err_gd)
    plt.show()
    y_hat = predict(w_star_gd, x_train)
    print("Accuracy: ", accuracy(y_hat, y_train))
```



Accuracy: 0.8225730443

/tmp/ipykernel_11714/3753579620.py:2: RuntimeWarning: overflow encountered in exp

return 1 / (1 + np.exp(-x))