

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

## MLE

```
In [ ]: def define_dataset(a, b, N, k, sigma):
    X = np.linspace(a, b, N)

    Phi = vander(X, k)

    theta_true = np.ones((k, ))

    Y = Phi @ theta_true
    gaussian_noise = np.random.normal(0, 1, Y.shape)
    Y = Y + sigma * gaussian_noise #Noisy Y

    D = (X, Y)

    return D

#Generalized Vandermonde Matrix
def vander(X, k):
    N = len(X)

    phi = np.zeros((N, k))

    for j in range(k):
        phi[:,j] = X**j

    return phi
```

```
In [ ]: def split_data(X, Y, percentage_train):

    N = len(X)
    Ntrain = int(percentage_train*N/100)

    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, Ytrain), (Xtest, Ytest)
```

```
In [ ]: #Degree of polynomial
k_chosen = (int) (input("Choose the degree of the polynomial: "))
```

```

#Input dataset
a = (int) (input("Choose an interval [a, b] --a: "))
b = (int) (input("Choose an interval [a, b] --b: "))

sigma = (float) (input("Choose the variance of the noise: "))

N = 100 #number of datapoints

X, Y = define_dataset(a, b, N, k_chosen, sigma)
D = (X, Y)

D_train, D_test = split_data(D[0], D[1], 70)
X_train, Y_train = D_train
X_test, Y_test = D_test

```

Pretend not to know the correct value of  $k$ . The task is to try guess it and use it to approximate the true solution  $\theta_{true}$  by MLE and MAP.

```

In [ ]: def f_MLE(X, Y):
        return lambda theta: 0.5 * (np.linalg.norm((vander(X, len(theta)) @ theta) - Y))**2

def grad_f_MLE(X, Y):
    return lambda theta: vander(X, len(theta)).T @ ((vander(X, len(theta)) @ theta) - Y)

def f_MAP(X, Y, lamda):
    return lambda theta: 0.5 * (np.linalg.norm((vander(X, len(theta)) @ theta) - Y))**2 + lamda * len(theta)

def grad_f_MAP(X, Y, lamda):
    return lambda theta: vander(X, len(theta)).T @ ((vander(X, len(theta)) @ theta) - Y) + lamda

```

```

In [ ]: def GD(grad_f, x0, kmax=100, tolf=1e-6, tolx=1e-6, alpha=1e-3):
    k = 0
    dim_m, dim_n = (kmax+1, x0.shape[0])
    x = np.empty((dim_m, dim_n))

    x[k]=x0

    conditions = True

    while (conditions and k < kmax):
        k = k+1

        x[k] = x[k-1]-alpha*grad_f(x[k-1])

        cond1 = np.linalg.norm(grad_f(x[k])) > tolf * grad_f(x[k-1]).all()
        cond2 = np.linalg.norm(x[k] - x[k-1]) > tolx * np.linalg.norm(x[k-1]).all()
        conditions = cond1 and cond2

    x = x[:k+1]

    return x[-1]

def SGD(grad_l, w0, D, batch_size, n_epochs, lamda=0, alpha=1e-3):
    X, Y = D
    N = X.shape[0]

```

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n_batch_per_epoch = N//batch_size
tot_batch = n_batch_per_epoch * n_epochs

w = np.array(w0)
w_vector = np.zeros((tot_batch, len(w0)))

for epoch in range(n_epochs):
    X_shuffle, Y_shuffle = shuffle_data(X, Y)

    for b in range (n_batch_per_epoch):
        n = b*batch_size
        m = (b+1)*batch_size

        Mx = X_shuffle[n:m]
        My = Y_shuffle[n:m]

        if lamda==0:
            gradient=grad_l(Mx, My)
        else:
            gradient=grad_l(Mx, My, lamda)

        w=w-alpha*gradient(w)
        w_vector[epoch*n_batch_per_epoch + b, :] = w

    return w_vector[-1]

def shuffle_data(X, Y):
    N = X.shape[0]
    indexes = np.arange(N)
    np.random.shuffle(indexes)

    X_shuffle = X[indexes]
    Y_shuffle = Y[indexes]

    return X_shuffle, Y_shuffle

```

```

In [ ]: def MLE(D, k_trial, mod):
    X, Y = D
    Phi_trial = vander(X, k_trial)

    if mod[0]=='N':
        #Normal equation
        A = Phi_trial.T @ Phi_trial
        b = Phi_trial.T @ Y
        try:
            L = scipy.linalg.cholesky(A, lower = True)
            y = scipy.linalg.solve_triangular(L, b, lower = True)
            theta_mle = scipy.linalg.solve_triangular(L.T, y)
        except:
            theta_mle = np.linalg.solve(Phi_trial.T @ Phi_trial, Phi_trial.T @ Y)

    elif mod[0]=='G':
        #Gradient Descent
        theta_mle = GD(grad_f_MLE(X, Y), np.zeros((k_trial,)))

    else:

```

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#Stochastic Gradient Descent
theta_mle = SGD(grad_f_MLE, np.zeros((k_trial, )), D, batch_size = 5, n_epochs=1000)

return theta_mle

```

```

In [ ]: theta_mle_normal = MLE(D, k_chosen, 'Normal equation')
theta_mle_gd = MLE(D, k_chosen, 'GD')
theta_mle_sgd = MLE(D, k_chosen, 'SGD')

print("Theta, MLE - Normal equation: ", theta_mle_normal)
print("Theta, MLE - GD: ", theta_mle_gd)
print("Theta, MLE - SGD: ", theta_mle_sgd)

```

```

Theta, MLE - Normal equation: [0.98171263 1.14624711 0.86958274 0.96888406]
Theta, MLE - GD: [1.06255607 1.06258762 0.92149537 0.80063846]
Theta, MLE - SGD: [1.05073984 0.68853411 0.52470793 0.42730751]

```

```

In [ ]: def polynomial_regression(X, k, theta):
    Phi = vander(X, k)
    return Phi @ theta

def error(D, k, theta):
    X, Y = D
    N = len(Y)

    f_theta = polynomial_regression(X, k, theta)

    return ((np.linalg.norm(f_theta - Y))**2) / N

```

For different values of K, plot the training datapoints and the test datapoints with different colors, and visualize (as a continuous line) the learnt regression model  $f_{\theta_{MLE}}(x)$ .

```

In [ ]: k_vector = [2, 4, 20, 60]
theta_mle_vector = []

for k in k_vector:
    theta_mle = MLE(D_train, k, "GD")
    theta_mle_vector.append(theta_mle)

fig, ax = plt.subplots(len(k_vector), figsize=(12, 15))

for i in range(len(k_vector)):

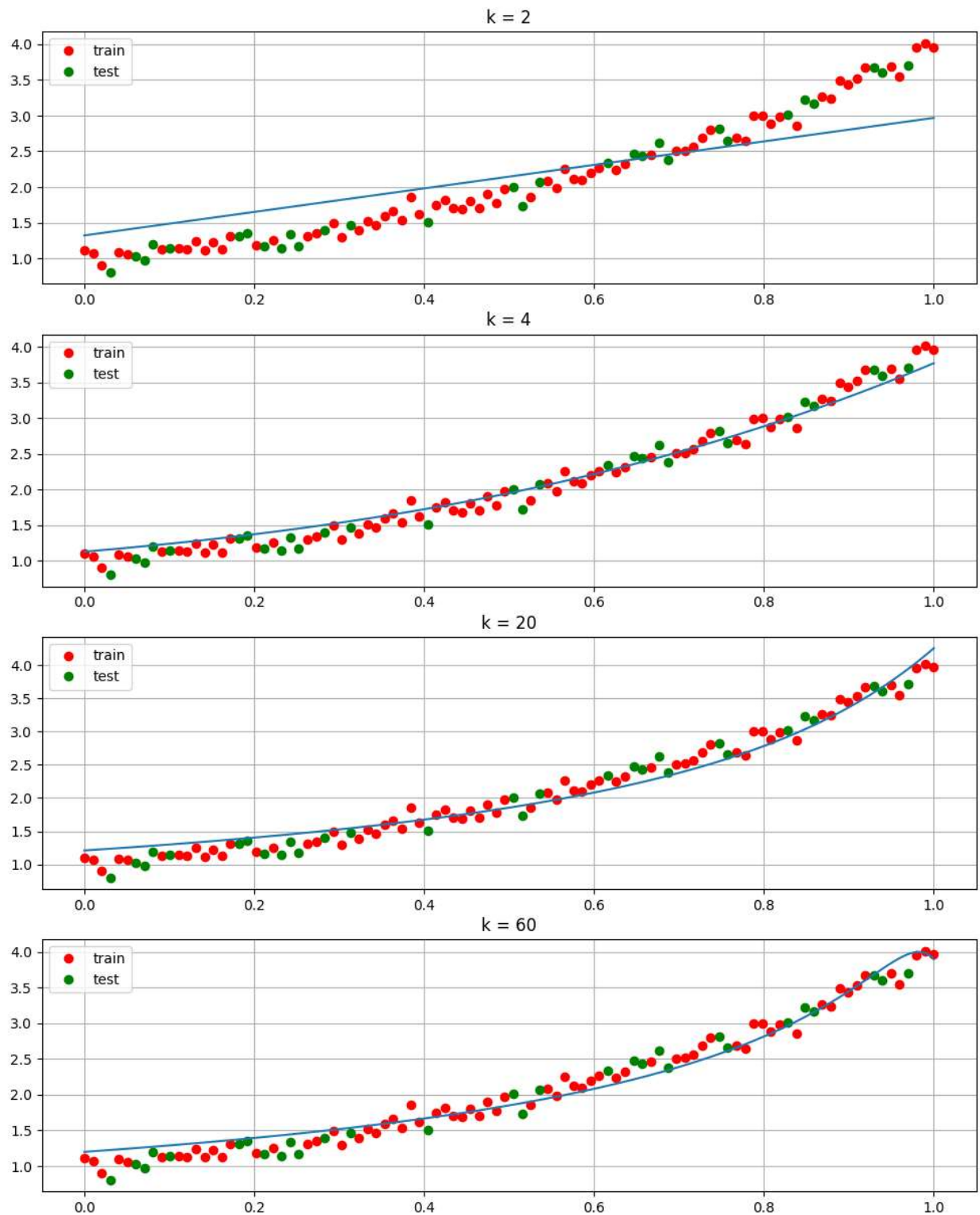
    theta = theta_mle_vector[i]
    k = k_vector[i]

    XX = np.linspace(a, b, 1000)
    YY = polynomial_regression(XX, k, theta)

    ax[i].set_title(f'k = {k}')
    ax[i].plot(X_train, Y_train, 'ro')
    ax[i].plot(X_test, Y_test, 'go')
    ax[i].legend(['train', 'test'])
    ax[i].plot(XX, YY)
    ax[i].grid()

```

```
plt.show()
```



For increasing values of  $K$  compute the training and test error. Plot the two errors with respect to  $K$ .

```
In [ ]: k_vector = np.arange(2, 21)

theta_vector = []
errors_train = []
```

```

errors_test = []

for k in k_vector:
    theta_mle = MLE(D_train, k, "GD")
    theta_vector.append(theta_mle)

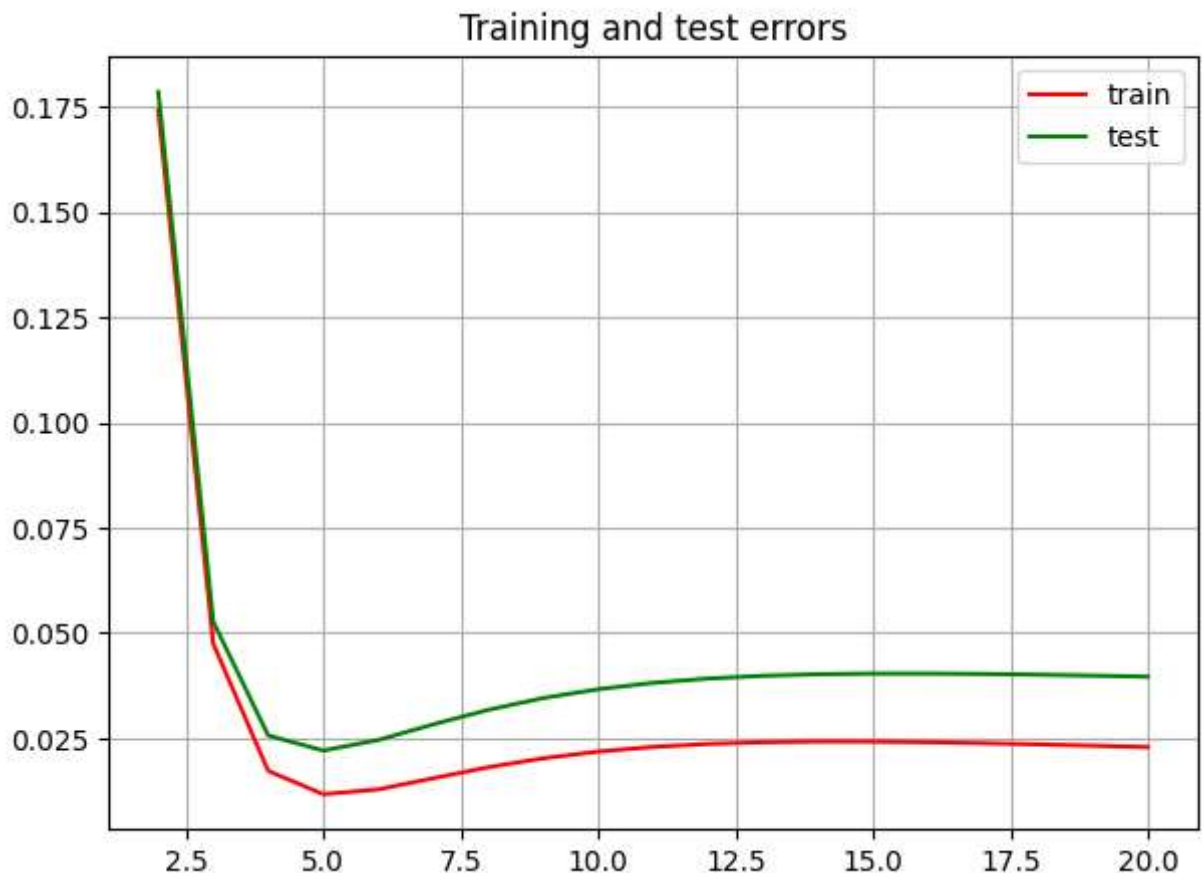
    training_error = error(D_train, k, theta_mle)
    errors_train.append(training_error)

    test_error = error(D_test, k, theta_mle)
    errors_test.append(test_error)

plt.figure(figsize=(7,5))
plt.title("Training and test errors")
plt.plot(k_vector, errors_train, color='red')
plt.plot(k_vector, errors_test, color='green')
plt.legend(['train', 'test'])
plt.grid()
plt.plot()

```

Out[ ]: []



## MAP

Write a function that returns the MAP solution. Note that the loss function can be optimized by GD, SGD or Normal Equations.

```
In [ ]: def MAP(D, k_trial, lambda, mod):
    X, Y = D

    Phi = vander(X, k_trial)

    if mod[0] == 'N':
        #Normal equation
        A = (Phi.T @ Phi) + (lambda * np.identity(k_trial))
        b = Phi.T @ Y

        try:
            L = scipy.linalg.cholesky(A, lower = True)
            y = scipy.linalg.solve_triangular(L, b, lower = True)
            theta_MAP = scipy.linalg.solve_triangular(L.T, y)
        except:
            theta_MAP = np.linalg.solve((Phi.T @ Phi) + (lambda * np.identity(k_trial)))

    elif mod[0] == 'G':
        #Gradient Descent
        theta_MAP = GD(grad_f_MAP(X, Y, lambda), np.zeros((k_trial, )))

    else:
        #Stochastic Gradient Descent
        theta_MAP = SGD(grad_f_MAP, np.zeros((k_trial, )), D, 5, 10, lambda)

    return theta_MAP
```

```
In [ ]: theta_map_normal = MAP(D, k_chosen, 1, 'Normal equation')
theta_map_gd = MAP(D, k_chosen, 1, 'GD')
theta_map_sgd = MAP(D, k_chosen, 1, 'SGD')

print("Theta, MAP, lambda = 1 - Normal equation: ", theta_map_normal)
print("Theta, MAP, lambda = 1 - GD: ", theta_map_gd)
print("Theta, MAP, lambda = 1 - SGD: ", theta_map_sgd)
```

```
Theta, MAP, lambda = 1 - Normal equation: [0.99902566 1.08570032 0.96566516 0.853176
34]
Theta, MAP, lambda = 1 - GD: [1.06972382 1.03545407 0.8910705 0.77146094]
Theta, MAP, lambda = 1 - SGD: [0.91067276 0.59374062 0.45132836 0.36691072]
```

For K lower, equal and greater than the correct degree of the test polynomial, plot the training datapoints and the test datapoints with different colors, and visualize (as a continuous line) the learnt regression model  $f_{\theta_{MAP}}(x)$  with different values of lambda.

```
In [ ]: k_vector = [2, 4, 10]
l_vector = [0, 1, 7]

theta_tot_k = []

for k in k_vector:

    theta_tot_l = []

    for l in l_vector:
        theta_map = MAP(D_train, k, l, "GD")
        theta_tot_l.append(theta_map)
```

```

theta_tot_k.append(theta_tot_l)

for i in range(len(k_vector)):
    k = k_vector[i]

    plt.figure(figsize=(20, 4))
    plt.suptitle(f'k = {k}')

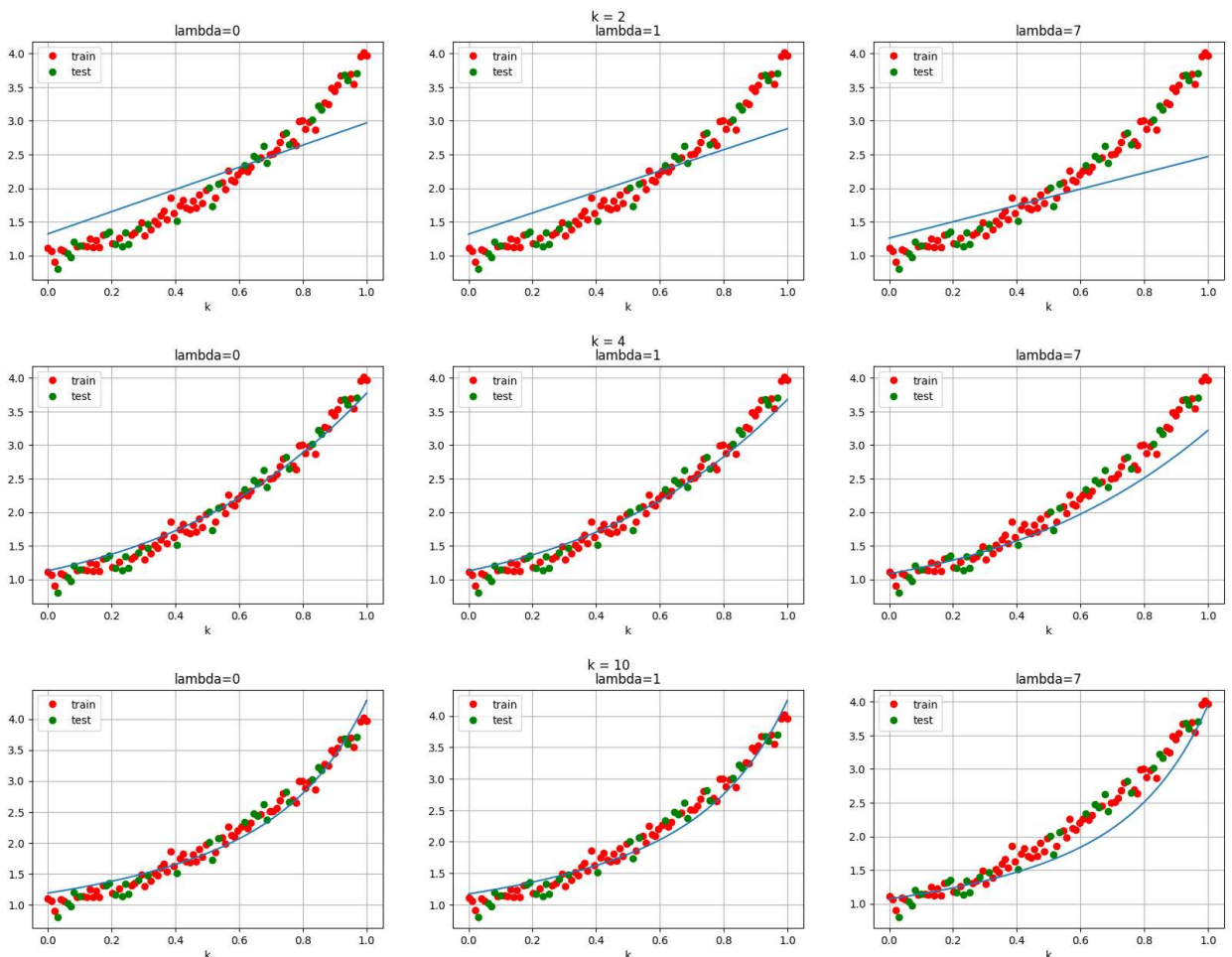
    for j in range(len(theta_tot_k[i])):
        theta = theta_tot_k[i][j]

        plt.subplot(1, len(theta_tot_k[i]), j+1)
        plt.title(f"lambda={l_vector[j]}")
        plt.xlabel('k')

        XX = np.linspace(a, b, 1000)
        YY = polynomial_regression(XX, k, theta)
        plt.plot(X_train, Y_train, 'ro')
        plt.plot(X_test, Y_test, 'go')
        plt.legend(['train', 'test'])
        plt.plot(XX, YY)
        plt.grid()

plt.show()

```



For increasing values of  $K$  compute the training and test error. Plot the two errors with respect to  $K$ .



```

In [ ]: k_vector = np.arange(2, 21)

theta_vector = []
errors_train = []
errors_test = []

lmbda = 1

for k in k_vector:
    theta_map = MAP(D_train, k, lmbda, "GD")
    theta_vector.append(theta_map)

    training_error = error(D_train, k, theta_map)
    errors_train.append(training_error)

    test_error = error(D_test, k, theta_map)
    errors_test.append(test_error)

plt.figure(figsize=(7,5))
plt.title("Training and test errors")
plt.plot(k_vector, errors_train, color='red')
plt.plot(k_vector, errors_test, color='green')
plt.legend(['train', 'test'])
plt.grid()
plt.plot()

```

Out[ ]: []



# MLE and MAP

For  $K$  being way greater than the correct degree of the polynomial, compute the MLE and MAP solution. Compare the test error of the two, for different values of  $\lambda$  (in the case of MAP).

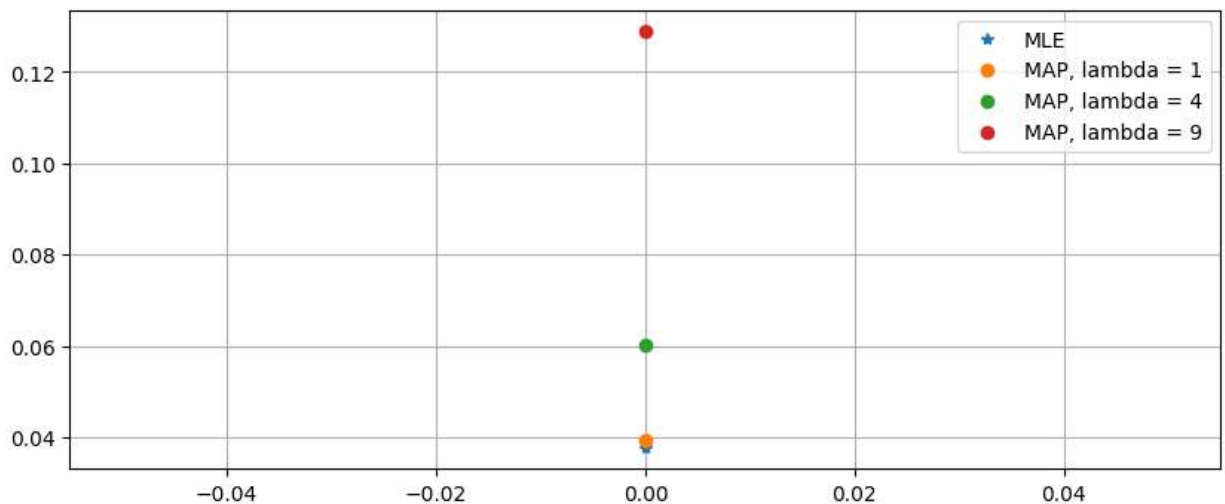
```
In [ ]: k_big = 70
l_vector = [1, 4, 9]

theta_mle = MLE(D_train, k_big, "GD")
thetas_map = [MAP(D_train, k_big, l, "GD") for l in l_vector]

mle_error = error(D_test, k_big, theta_mle)
map_errors = [error(D_test, k_big, theta_map) for theta_map in thetas_map]

legend_mle = ['MLE']
legend_map = ['MAP, lambda = ' + str(l) + '' for l in l_vector]
legend = legend_mle + legend_map

plt.figure(figsize=(10,4))
plt.plot(mle_error, '*')
for i in range(len(l_vector)):
    plt.plot(map_errors[i], 'o')
plt.legend(legend)
plt.grid()
plt.show()
```



For  $K$  greater than the true degree of the polynomial, define the relative error and compute it for MLE and MAP for increasing values of  $K$ .

```
In [ ]: def err_theta(theta, k):
    theta_true = np.ones((k,))
    diff = len(theta) - k
    if(diff > 0):
        theta_true = np.concatenate(theta_true, np.zeros(diff))
    return np.linalg.norm(theta - theta_true) / np.linalg.norm(theta_true)
```

```
In [ ]: k_vector = np.arange(2, 61)
lambda = 1
```

```

theta_mle_error_tot_k = np.asarray([err_theta(MLE(D_train, k, "GD"), k) for k in k_vec])
theta_map_error_tot_k = np.asarray([err_theta(MAP(D_train, k, lambda, "GD"), k) for k in k_vec])
diff = np.linalg.norm(theta_mle_error_tot_k[:, np.newaxis] - theta_map_error_tot_k[:, np.newaxis], axis=0)

legend = ['MLE', 'MAP']

plt.figure(figsize=(12, 5))

plt.subplot(1, 2, 1)
plt.title("MLE and MAP errors")
plt.plot(k_vector, theta_mle_error_tot_k, color='red')
plt.plot(k_vector, theta_map_error_tot_k, color='green')
plt.xlabel('k')
plt.legend(legend)
plt.grid()

plt.subplot(1, 2, 2)
plt.title("Difference between MLE and MAP errors")
plt.plot(k_vector, diff)
plt.xlabel('k')
plt.grid()

plt.show()

```

