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

Polynomial regression as linear least squares

From the knowledge of a sample of pair of scalar values $\{a_i, y_i\}_{i=1}^n$, we would like to predict the relation between x and y. One simple way to go beyond linear regression is to consider polynomial regression: for example we could try to model y as a polynomial of degree 3 of a. We would look for $(x_0, x_1, x_2, x_3) \in \mathbb{R}^4$ such that the values a_i and y_i are linked as $y_i \simeq x_0 + x_1 a_i + x_2 a_i^2$.

This problem can be mapped to linear regression by considering that we have for each a a feature vectors of dimension $d+1$ when considering the fit of a polynomial of degree d. This feature vector is $(1, a, a^2, \cdots, a^d)$. Such that the full data matrix is

$$A = \begin{bmatrix} 1 & a_1 & \cdots & a_1^d \\ 1 & a_2 & \cdots & a_2^d \\ \vdots & \vdots & \vdots & \vdots \\ 1 & a_n & \cdots & a_n \end{bmatrix} \in \mathbb{R}^{n\times(d+1)}.$$

As a exercise below we will consider data that was created from a polynomial of dimension 3, to which noise is added. Assuming that we do not know the degree of the generated polynomial, we will try to fit with $d = 5$ and $d = 2$ and investigate ridge regression.

In [ ]:
```
## Helper functions to setup the problem
def get_data_mat(a, deg):
    """
    Inputs:
    a: (np.array of size N)
    deg: (int) max degree used to generate the data matrix

    Returns:
    A: (np.array of size N x (deg_true + 1)) data matrix
    """
    A = np.array([a ** i for i in range(deg + 1)]).T
    return A

def draw_sample(deg_true, x, N, eps=0):
    """
    Inputs:
    deg_true: (int) degree of the polynomial g
    a: (np.array of size deg_true) parameter of g
    N: (int) size of sample to draw
    eps: noise level

    Returns:
    x: (np.array of size N)
    y: (np.array of size N)
    """
```

```
    a = np.sort(np.random.rand(N))
    A = get_data_mat(a, deg_true)
    y = A @ x + eps * np.random.randn(N)
    return a, y
```

(a) Complete the three functions below to obtain

- the least square estimator x^{LS}
- the ridge estimator x^{Ridge}
- the mean square error $\|Ax - y\|^2/n$

In [ ]:

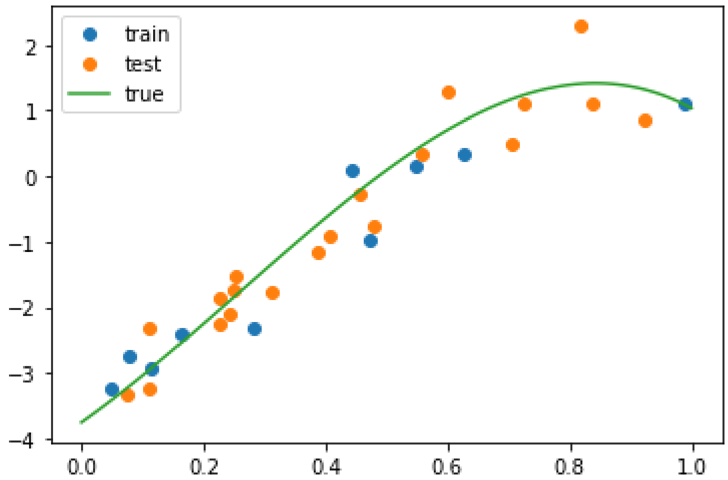
```
def least_square_estimator(A, y):
    x_ls = np.linalg.inv((A.transpose()) @ A) @ (A.transpose()) @ y
    return np.array(x_ls)

def ridge_estimator(A, y, lbd):
    A_t = A.transpose()
    A_t_A = (A_t @ A)
    lbd_term = (lbd * np.identity(np.shape(A_t_A)[0]))
    x_ridge_inv = np.linalg.inv(A_t_A + lbd_term)
    x_ridge_2 = A_t @ y
    x_ridge = x_ridge_inv @ x_ridge_2
    return np.array(x_ridge)

def mean_squared_error(x, A, y):
    norm = (np.linalg.norm((A @ x) - y)) ** 2
    mse = norm / len(y)
    return mse
```

In [ ]:

```
# This cells generates the data - for your submission do not change it.
# But for your own curiosity, do not hesistate to investigate what is going on w

np.random.seed(45) # fixing seed so everyone should see the same data
N = 10
deg_true = 3 # degree of true polynomial
eps = 0.5 # noise amplitude
x_true = np.array([-3.75307359,  6.58178662,  6.23070014, -8.02457871])

# radom input data
a_tr, y_tr = draw_sample(deg_true, x_true, N, eps=eps) # training data
a_te, y_te = draw_sample(deg_true, x_true, 2 * N, eps=eps) # testing data

a_plot = np.linspace(0, 1, 100)
A_plot = get_data_mat(a_plot, deg_true)
plt.plot(a_tr, y_tr,'o', label='train')
plt.plot(a_te, y_te,'o', label='test')
plt.plot(a_plot, A_plot @ x_true,'-', label='true')
plt.legend()
```

Out[ ]:

```
<matplotlib.legend.Legend at 0x7fbd01a6b340>
```



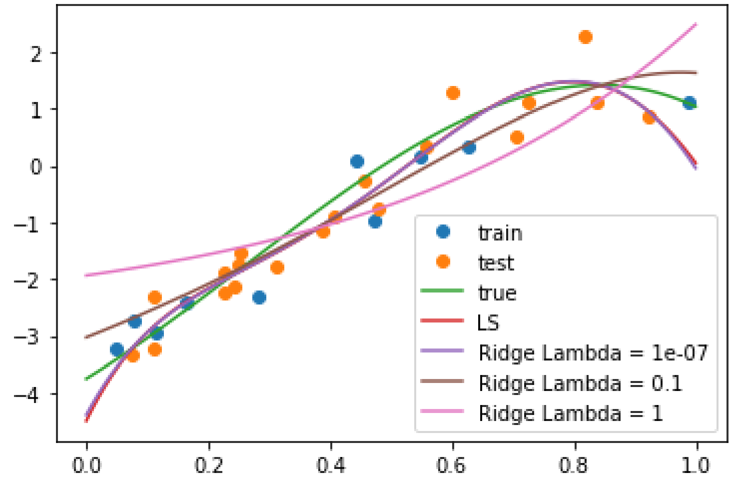
(b) Complete the code below to visualize the prediction of x^{LS} and x^{Ridge} for λ in $[1e-7, 0.1, 1]$, using in all cases a prediction model of degree 5. The output of the cell should be a plot as above, where you added three lines of predictions for all values of $a \in [0,1]$: line LS, line ridge $\lambda = 1e-7$, line ridge $\lambda = 0.1$, line ridge $\lambda = 1$.

In [ ]:

```
a_plot = np.linspace(0,1,100)
A_plot = get_data_mat(a_plot, deg_true)
plt.plot(a_tr, y_tr,'o', label='train')
plt.plot(a_te, y_te,'o', label='test')
plt.plot(a_plot, A_plot @ x_true,'-', label='true')

deg_pred = 5

A_tr = get_data_mat(a_tr, deg_pred)
A_te = get_data_mat(a_te, deg_pred)

x_ls = least_square_estimator(A_te, y_te)

A_plot = get_data_mat(a_plot, deg_pred)
plt.plot(a_plot, A_plot @ x_ls, label='LS')

for lbd in [1e-7, 0.1, 1]:
   label = 'Ridge Lambda = ' + str(lbd)
   plt.plot(a_plot, A_plot @ ridge_estimator(A_te, y_te, lbd), label=label)
   pass
plt.legend()
```

Out[ ]:

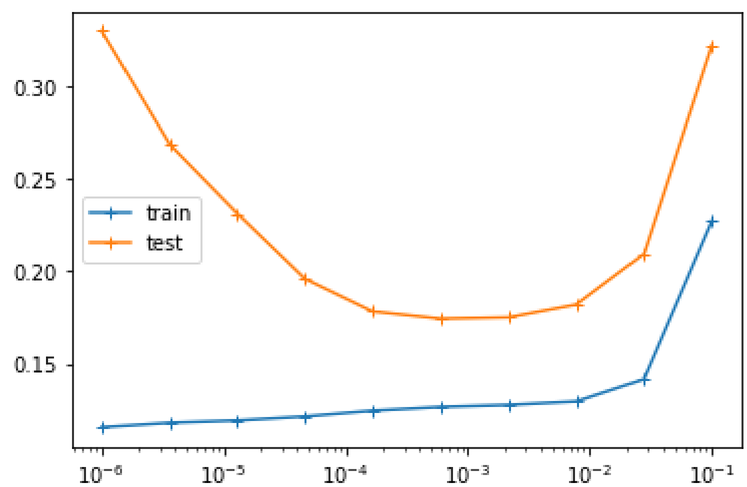
```
<matplotlib.legend.Legend at 0x7fbce181bdc0>
```



(c) Use the `mean_squared_error` to make a plot of the training error and the test error as a function of λ as we have seen in the lecture (range given below). Which value of λ would you choose? Does that align with your intuition from the plots above?

In [ ]:
```
tr_mse = []
te_mse = []
lbds = np.logspace(-6, -1, 10)
for lbd in lbds:
    ridge_train = ridge_estimator(A_tr, y_tr, lbd)
    tr_mse.append(mean_squared_error(ridge_train, A_tr, y_tr))
    te_mse.append(mean_squared_error(ridge_train, A_te, y_te))

plt.plot(lbds, tr_mse, '-+', label='train')
plt.plot(lbds, te_mse,'-+', label='test')
plt.xscale('log')
plt.legend()
```

Out[ ]:
```
<matplotlib.legend.Legend at 0x7fbce1a13850>
```

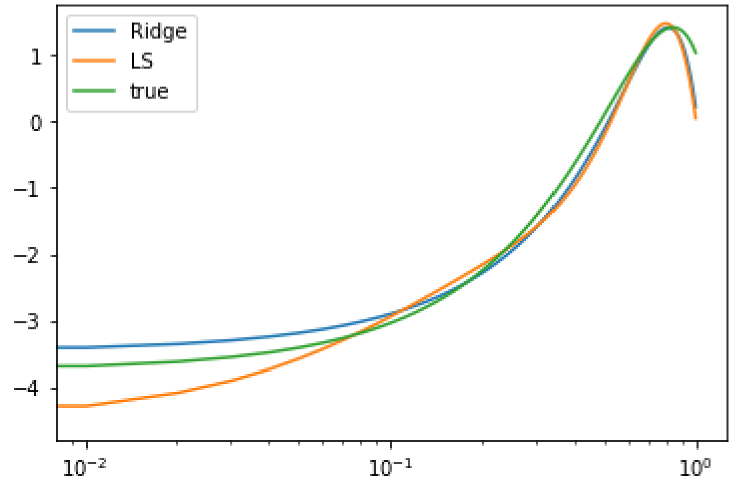


(d) For the optimal value of λ compare x^{LS}, x^{Ridge} and x^{true}.

In [ ]:
```
plt.plot(a_plot, A_plot @ ridge_estimator(A_te, y_te, 0.001), label='Ridge')
plt.plot(a_plot, A_plot @ x_ls, label='LS')
a_plot = np.linspace(0,1,100)
A_plot = get_data_mat(a_plot, deg_true)
```

```
plt.plot(a_plot, A_plot @ x_true,'-', label='true')
plt.xscale('log')
plt.legend()
```

Out[ ]: <matplotlib.legend.Legend at 0x7fbcd1cc7c70>

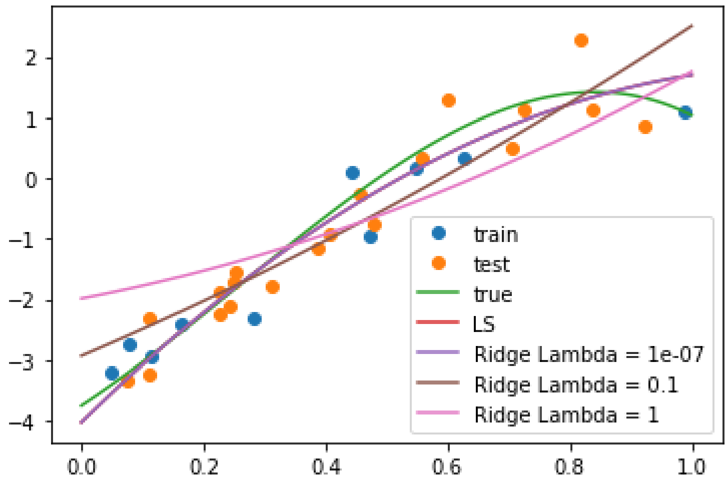


(e) Repeat the same operation with a fitting model of degree 2 (`deg_pred=2`). What are your findings related to the optimal degree of regularizations in this case?

In [ ]:

```
### PART B ###

a_plot = np.linspace(0,1,100)
A_plot = get_data_mat(a_plot, deg_true)
plt.plot(a_tr, y_tr,'o', label='train')
plt.plot(a_te, y_te,'o', label='test')
plt.plot(a_plot, A_plot @ x_true,'-', label='true')

deg_pred = 2

A_tr = get_data_mat(a_tr, deg_pred)
A_te = get_data_mat(a_te, deg_pred)

x_ls = least_square_estimator(A_te, y_te)

A_plot = get_data_mat(a_plot, deg_pred)
plt.plot(a_plot, A_plot @ x_ls, label='LS')

for lbd in [1e-7, 0.1, 1]:
   label = 'Ridge Lambda = ' + str(lbd)
   plt.plot(a_plot, A_plot @ ridge_estimator(A_te, y_te, lbd), label=label)
   pass
plt.legend()
```

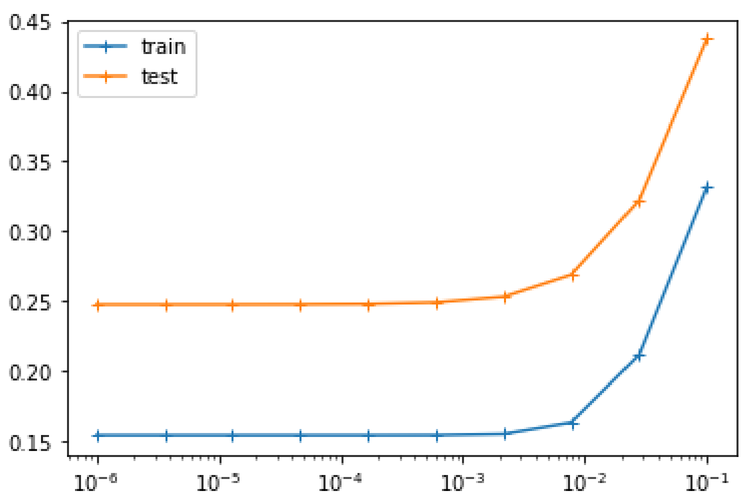
Out[ ]: <matplotlib.legend.Legend at 0x7fbcd1f08310>



In [ ]:

```
### PART C ###
tr_mse = []
te_mse = []
lbds = np.logspace(-6, -1, 10)
for lbd in lbds:
    ridge_train = ridge_estimator(A_tr, y_tr, lbd)
    tr_mse.append(mean_squared_error(ridge_train, A_tr, y_tr))
    te_mse.append(mean_squared_error(ridge_train, A_te, y_te))

plt.plot(lbds, tr_mse, '-+', label='train')
plt.plot(lbds, te_mse,'-+', label='test')
plt.xscale('log')
plt.legend()
```

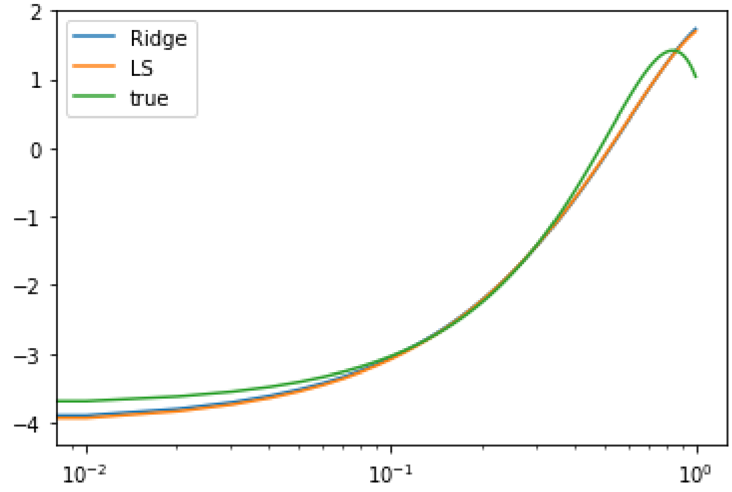
Out[ ]: <matplotlib.legend.Legend at 0x7fbce1d29d90>



In [ ]:

```
### PART D ###
plt.plot(a_plot, A_plot @ ridge_estimator(A_te, y_te, 0.001), label='Ridge')
plt.plot(a_plot, A_plot @ x_ls, label='LS')
a_plot = np.linspace(0,1,100)
A_plot = get_data_mat(a_plot, deg_true)
plt.plot(a_plot, A_plot @ x_true,'-', label='true')
plt.xscale('log')
plt.legend()
```

Out[ ]: <matplotlib.legend.Legend at 0x7fbce1ee3280>



It appears that the regularization term does not help quite as much in the case of an order two polynomial solution. The plot generated affirms the idea of choosing a regularization parameter with the smallest value.