Kernel Regression

Given a training dataset $\{x_i, y_i\}_{i=1}^n$, kernel regression approximates the unknown nolinear relation between x and y with a function of form

$$y \approx f(x; w) = \sum_{i=1}^{n} w_i k(x, x_i),$$

where $k(x, x')$ is a positive definite kernel specified by the users, and w_i is a set of weights. We will use the simple Gaussian radius basis funciton (RBF) kernel,

$$k(x, x') = exp(-\frac{||x - x'||^2}{2h^2}),$$

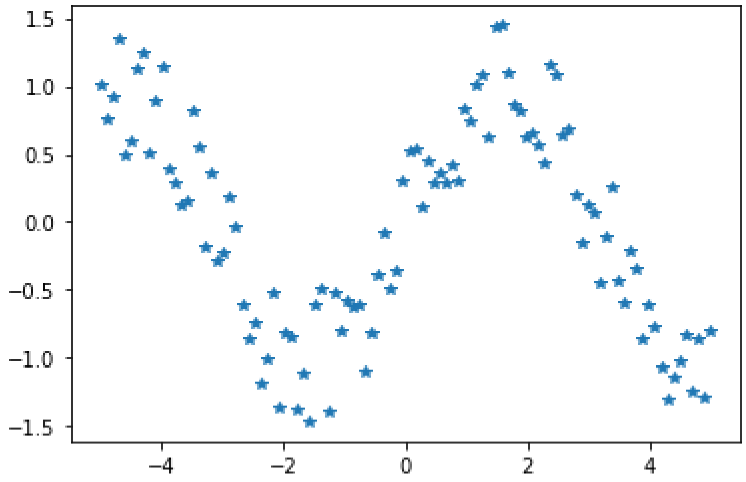
where h is a bandwith parameter.

Step 1. Simulate a 1-dimensional dataset

In [1]:

```
import numpy as np
import matplotlib
import matplotlib.pyplot as plt
%matplotlib inline

np.random.seed(100)

### Step 1: Simulate a simple 1D data ###
xTrain = np.expand_dims(np.linspace(-5, 5, 100), 1)  # 100*1
yTrain = np.sin(xTrain) + 0.5*np.random.uniform(-1, 1, size=xTrain.shape) ## 100
*1

print('xTrain shape', xTrain.shape, 'yTrain shape', yTrain.shape)
plt.plot(xTrain, yTrain, '*')
plt.show()
```

```
xTrain shape (100, 1) yTrain shape (100, 1)
```



Now we have a dataset with 100 training data points. Let us calculate the kernel function.

Step 2. Kernel function

Your task is to complete the following rbf_kernel function that takes two sets of points X (of size n) and X' (of size m) and the bandwidth h and ouputs their pairwise kernel matrix $K = [k(x_i, x_j)]_{ij}$, which is of size $n \times m$. We will represent input data as matrices, with $X = [x_i]_{i=1}^n \in R^{n \times 1}$ denoting the input features and $Y = [y_i]_{i=1}^n \in R^{n \times 1}$ the input labels.)

In [2]:

```
"""
    calcuating kernel matrix between X and Xp
"""
def rbf_kernel(X, Xp, h):
    # X: n*1 matrix
    # Xp: m*1 matrix
    # h: scalar value

    ## TODO: please calculate the kernel matrix in the following:
    # (hint: you can write your own pairwise distance function, or cipy.spatial.
distance.cdist)

    K = np.array([[np.exp(-(x_p - x) ** 2 / (2 * h ** 2)) for x_p in Xp] for x i
n X]).squeeze()

    return K #n*m



### evaluation: if your implementation is correct, you should expect the output
is a 2X3 matrix
# [[0.60653066 1.          0.60653066]
# [0.13533528 0.60653066 1.          ]]
k_test = rbf_kernel(np.array([[2],[1]]), np.array([[3],[2],[1]]), 1)
print(k_test)
```

```
[[0.60653066 1.         0.60653066]
 [0.13533528 0.60653066 1.        ]]
```

Step 3. The median trick for bandwith

The choice of the bandwidth h A common way to set the bandwith h in practice is the so called median trick, which sets h to be the median of the pairwise distance on the training data, that is

$$h_{med} = median(\{||x_i - x_j|| : i \neq j, \quad i, j = 1, \ldots, n\}).$$

- Task: Compelete the median distance function.

In [3]:

```
from scipy.spatial import distance

def median_distance(X):
    # X: n*1 matrix

    #TODO: Calculate the median of the pairwise distance of $X$ below
    #(hint: use '[dist[i, j] for i in range(len(X)) for j in range(len(X)) if i
!= j]' to remove the diagonal terms; use np.median)
    distances = [np.abs(X[i] - X[j]) for i in range(len(X)) for j in range(i+1,
len(X))] # no need to duplicate X[i], X[j] distance to calculate the median
    h = np.median(distances)
    return h


### Test your functions
#evaluation: if your implementation is correct, your answer should be [2.0]
h_test = median_distance(np.array([[1],[2],[4]]))
print(h_test)
```

```
2.0
```

Step 4. Kernel regression

The weights w_i are estimated by minimizing a regularized mean square error:

$$\min_{w} \left(\sum_{i=1}^{n} (y_i - f(x_i; w))^2 \right) + \beta w^\top K w,$$

where w is the column vector formed by $w = [w_i]_{i=1}^{n}$ and K is the kernel matrix.

- Please derive the optimal solution of w using matrix inverseion (no need to show the work)
- Complete the following function to implement the calculation of w

In [4]:

```
def kernel_regression_fitting(xTrain, yTrain, h, beta=1):
    # X: input data, numpy array, n*1
    # Y: input labels, numpy array, n*1


    # TODO: calculate W below (it is a n*1 matrix)
    K = rbf_kernel(xTrain, xTrain, h)
    W = np.linalg.inv(K + beta * np.eye(K.shape[0])) @ yTrain

    return W

### evaluating your code, the shape should be (100, 1) (check the values yoursel
f)
h = median_distance(xTrain)
W_test = kernel_regression_fitting(xTrain, yTrain, h)
print(W_test.shape)
```

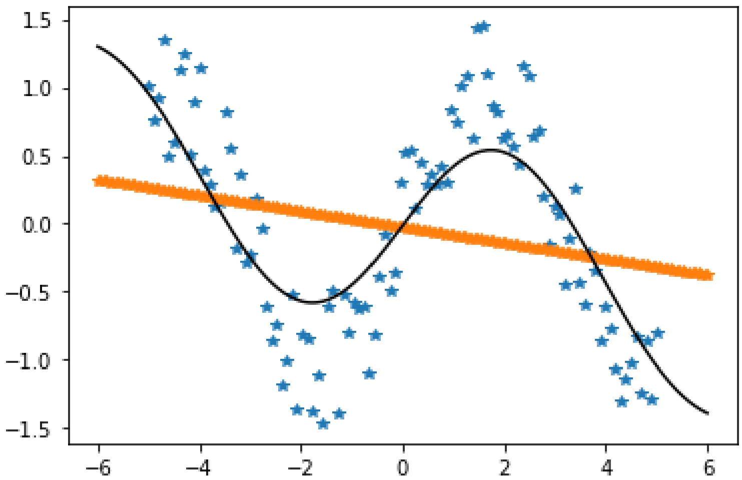
```
(100, 1)
```

Step 5. Evaluation and Cross Validation

We now need to evaluate the algorithm on the testing data and select the hyperparameters (bandwidth and regularization coefficient) using cross validation

In [5]:

```
# Please run and read the following base code

def kernel_regression_fit_and_predict(xTrain, yTrain, xTest, h, beta):

    #fitting on the training data
    W = kernel_regression_fitting(xTrain, yTrain, h, beta)

    # computing the kernel matrix between xTrain and xTest
    K_xTrain_xTest = rbf_kernel(xTrain, xTest, h)

    # predict the label of xTest
    yPred = np.dot( K_xTrain_xTest.T, W)
    return yPred

# generate random testing data
xTest = np.expand_dims(np.linspace(-6, 6, 200), 1) ## 200*1


beta = 1.
# calculating bandwith
h_med = median_distance(xTrain)
yHatk = kernel_regression_fit_and_predict(xTrain, yTrain, xTest, h_med, beta)


# we also add linear regression for comparision
from sklearn.linear_model import LinearRegression
lr = LinearRegression()
lr.fit(xTrain, yTrain)
yHat = lr.predict(xTest) # prediction

# visulization
plt.plot(xTrain, yTrain, '*')
plt.plot(xTest, yHat, '*')
plt.plot(xTest, yHatk, '-k')
plt.show()
```



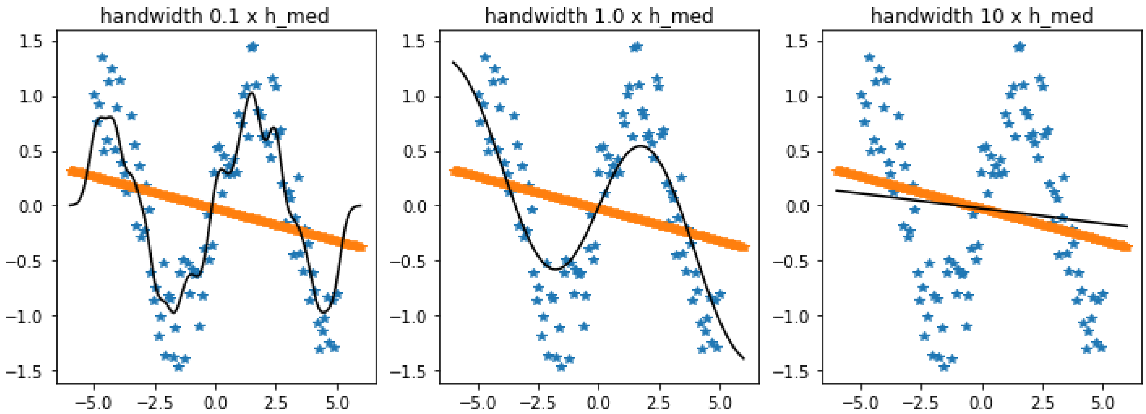
Step 5.1. Impact of bandwith

Run the kernel regression with regularization coefficient $\beta = 1$ and bandwidth $h \in \{0.1h_{med}, h_{med}, 10h_{med}\}$.

- Task: Show the curve learned by different h. Comment on how h influences the smoothness of h.

In [6]:

```
### fitting on the training data ###
beta = 1.

plt.figure(figsize=(12, 4))
for i, coff in enumerate([0.1, 1., 10]):
    plt.subplot(1, 3, i+1)

    ### TODO: run kernel regression with bandwith h = coff * h_med.
    yHatk_i = yHatk = kernel_regression_fit_and_predict(xTrain, yTrain, xTest, c
off*h_med, beta)

    # visulization
    plt.plot(xTrain, yTrain, '*')
    plt.plot(xTest, yHat, '*')
    plt.plot(xTest, yHatk_i, '-k')
    plt.title('handwidth {} x h_med'.format(coff))

plt.show()
```



Answer: smaller bandwidth makes approximated function to predict smaller variations in the data and makes it less smoother.

Step 5.2. Cross Validation (CV)

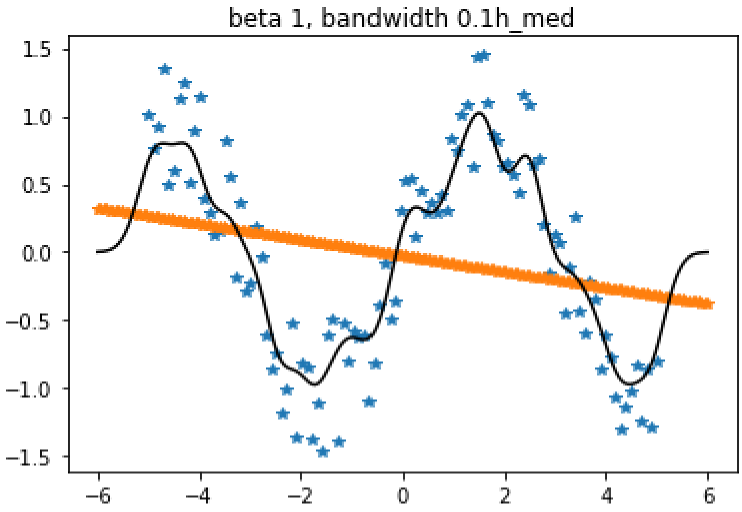
Use 5-fold cross validation to find the optimal combination of h and β within $h \in \{0.1h_{med}, h_{med}, 10h_{med}\}$ and $\beta \in \{0.1, 1\}$.

- Task: complete the code of cross validation and find the best h and β. Plot the curve fit with the optimal hyperparameters.

In [7]:

```
best_beta, best_coff = 1., 1.
best_mse = 1e8
for beta in [0.1, 1]:
    for coff in [0.1, 1., 10.]:
        # 5-fold cross validation
        max_fold = 5
        mse = []
        for i in range(max_fold):

            ##TODO: calculate the index of the training/testing partition within 5 fold CV.
            # (hint: set trnIdx to be these index with idx%max_fold!=i, and testIdx with idx%max_fold==i)
            trnIdx = [k for k in range(len(xTrain)) if k % max_fold != i]
            testIdx = [k for k in range(len(xTrain)) if k % max_fold == i]

            i_xTrain, i_yTrain = xTrain[trnIdx], yTrain[trnIdx]
            i_xValid, i_yValid = xTrain[testIdx], yTrain[testIdx]


            ##TODO: run kernel regression on (i_xTrain, i_yTrain) and calculate the mean square error on (i_xValid, i_yValid)
            h = coff * median_distance(i_xTrain)
            W = kernel_regression_fitting(i_xTrain, i_yTrain, h, beta)
            K_xx = rbf_kernel(i_xTrain, i_xValid, h)
            i_yPred = np.dot(K_xx.T, W)
            mse.append((i_yValid - i_yPred)**2)

        mse = np.mean(mse)

        # keep track of the combination with the best MSE
        if mse < best_mse:
            best_beta, best_coff = beta, coff
            best_mse = mse

print('Best beta', best_beta, 'Best bandwith', '{}*h_med'.format(best_coff), 'mse', best_mse)

# bandwith
h = best_coff * median_distance(xTrain)
yHatk_i = kernel_regression_fit_and_predict(xTrain, yTrain, xTest, h, best_beta)

# visulization
plt.plot(xTrain, yTrain, '*')
plt.plot(xTest, yHat, '*')
plt.plot(xTest, yHatk_i, '-k')
plt.title('beta {}, bandwidth {}h_med'.format(best_beta, best_coff))
plt.show()
```

```
Best beta 1 Best bandwith 0.1*h_med mse 0.11166229355896191
```



In [ ]: