Exercise 01

Kernel Methods in Machine Learning (CS-E4830)

Tasks: 1. [Implement kernel matrix calculation](#task_1) 1. [Linear kernel](#task_1_a) (**1 Point**) 2. [Gaussian kernel](#task_1_b) (**2 Point**) 2. [Implement the Parzen Window Classifier](#task_2) (**2 Point**) 3. [Application of the Parzen Window Classifier](#task_3) 1. [Implement the hyper parameter optimization](#task_3_a) (**2 Point**) 2. [Plot validation score for different hyper parameters](#task_3_b)(**1 Point**)

Optional Tasks: 4. [Model visualization: Non-linear vs. Linear](#task_4) (**no points**)

Version: 1.0

Version history:

- 1.0: Initial version

Please add your student number and email address to the notebook into the corresponding cell.

EMAIL: christian.segercrantz@aalto.fi

STUDENT_NUMBER: 481056

Import required python packages

All tasks in this exercise can be solved by using only function and packages imported below. Please **do not** use any other imports.

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.colors as colors
plt.set_cmap("RdBu_r")

from sklearn.base import BaseEstimator, ClassifierMixin
from sklearn.datasets import make_blobs, make_moons
from sklearn.model_selection import KFold, ParameterGrid, BaseCrossValidator, train_tes
t_split
from sklearn.base import clone
```

```
<Figure size 432x288 with 0 Axes>
```

1. Kernel matrix calculation

Your task is to **implement two functions to calculate Linear- and Gaussian-kernel matrices** for two sets of feature vectors $\mathbf{X}_A \in \mathbb{R}^{n_A \times d}, \mathbf{X}_B \in \mathbb{R}^{n_B \times d}$, where d is the dimension of the feature vectors, and n_a and n_B are the number of examples in set A respectively B.

A. Linear kernel (1 Point)

Task: Implement missing code parts of the function calculation the linear kernel matrix given two feature vector matrices $\mathbf{X}_A$ and $\mathbf{X}_B$. The resulting kernel matrix $\mathbf{K}_{lin}$ must have dimension $n_A \times n_B$. For a single entry in the kernel matrix it must hold:

$$[\mathbf{K}_{lin}]_{ij} = \kappa_{lin}(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle,$$

with $\mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^d$ being two examples from set A respecively B.

In [2]:

```python
def linear_kernel(X_A, X_B=None):
    """
    Calculate linear kernel matrix between two sets of feature-vectors, so that:

        k_ij = <x_i, x_j>

    :param X_A: array-like, shape=(n_samples_A, d), feature-matrix of set A
    :param X_B: array-like, shape=(n_samples_B, d), feature-matrix of set B or None, th
an Y = X

    :return: array-like, shape=(n_samples_A, n_samples_B), kernel matrix
    """
    if X_B is None:
        X_B = X_A

    K_AB = X_A @ X_B.T

    return K_AB
```

In [3]:

```
X_A = np.array([[1], [2], [3], [4]])
X_B = np.array([[0], [2], [1]])

# Test size
np.testing.assert_equal(linear_kernel(X_A, X_B).shape, (4, 3))
np.testing.assert_equal(linear_kernel(X_A).shape, (4, 4))

# Test values
np.testing.assert_equal(linear_kernel(X_A)[0, 0], 1)
np.testing.assert_equal(linear_kernel(X_A)[1, 1], 4)
np.testing.assert_equal(linear_kernel(X_A)[0, 2], 3)
np.testing.assert_equal(linear_kernel(X_A)[2, 0], 3)

np.testing.assert_equal(linear_kernel(X_A, X_B)[0, 0], 0)
np.testing.assert_equal(linear_kernel(X_A, X_B)[0, 1], 2)

# Test performance
import time
time_tolerance = 1  # in seconds
size = 3000

t0 = time.time()
a = linear_kernel(np.random.rand(size), np.random.rand(size))
t1 = time.time()
total = t1 - t0
print('Time to run with size {} = {:.4f} seconds'.format(size, total))
assert total < time_tolerance, 'Time limit exceeded'
```

```
Time to run with size 3000 = 0.0009 seconds
```

B. Gaussian kernel (1 Point)

Task: Implement missing code parts of the function calculation the Gaussian kernel matrix given two feature vector matrices $\mathbf{X}_A$ and $\mathbf{X}_B$. The resulting kernel matrix $\mathbf{K}_{gau}$ must have dimension $n_A \times n_B$. For a single entry in the kernel matrix it must hold:

$$[\mathbf{K}_{gau}]_{ij} = \kappa_{gau}(\mathbf{x}_i, \mathbf{x}_j) = \exp\left(-\frac{\|\mathbf{x}_i - \mathbf{x}_j\|^2}{2\sigma^2}\right)$$

with $\mathbf{x}_i, \mathbf{x}_j \in \mathbb{R}^d$ being two examples from set A respecively B, and $\gamma > 0$ being the bandwidth parameter.

In [4]:

```
def gaussian_kernel(X_A, X_B=None, sigma=None):
    """
    Calculate the Gaussian kernel matrix, so that

        k_ij = exp(-||x_i - x_j||^2 / (2 * sigma^2))

    :param X_A: array-like, shape=(n_samples_A, n_features), feature-matrix of set A
    :param X_B: array-like, shape=(n_samples_B, n_features), feature-matrix of set B or
None, than X_B = X_A
    :param sigma: scalar, bandwidth parameter

    :return: array-like, shape=(n_samples_A, n_samples_B), kernel matrix
    """
    if X_B is None:
        X_B = X_A

    n_A = X_A.shape[0]
    n_B = X_B.shape[0]

    if sigma is None:
        sigma = np.sqrt(X_A.shape[1] / 2.0)

    X_A_n, X_A_m = X_A.shape
    X_B_n, Y_B_m = X_B.shape

    X_A_sqrd = np.power(X_A, 2) @ np.ones((X_A_m, X_B_n))
    X_B_sqrd = np.ones((X_A_n, Y_B_m)) @ np.power(X_B, 2).T
    X_A_X_B = X_A @ X_B.T

    K_AB = np.exp(-(X_A_sqrd + X_B_sqrd - 2*X_A_X_B)/(2*sigma**2))
    #print("Res:\n", K_AB)

    return K_AB
```

In [5]:

```
X_A = np.array([[1], [2], [3], [4]])
X_B = np.array([[0], [2], [1]])

# Test size
np.testing.assert_equal(gaussian_kernel(X_A, X_B).shape, (4, 3))
np.testing.assert_equal(gaussian_kernel(X_A).shape, (4, 4))

# Test values
np.testing.assert_equal(gaussian_kernel(X_A, sigma=1)[0, 0], 1)
np.testing.assert_equal(gaussian_kernel(X_A, sigma=1)[1, 1], 1)
np.testing.assert_equal(gaussian_kernel(X_A, sigma=1)[0, 2], np.exp(-2))
np.testing.assert_equal(gaussian_kernel(X_A, sigma=1)[2, 0], np.exp(-2))

np.testing.assert_equal(gaussian_kernel(X_A, X_B, sigma=1)[0, 0], np.exp(-0.5))
np.testing.assert_equal(gaussian_kernel(X_A, X_B, sigma=1)[0, 1], np.exp(-0.5))

# Test performance
import time
time_tolerance = 1  # in seconds
size = 3000
features = 10

t0 = time.time()
a = gaussian_kernel(np.random.rand(size, features), np.random.rand(size, features))
t1 = time.time()
total = t1 - t0
print('Time to run with size {} = {:.4f} seconds'.format(size, total))
assert total < time_tolerance, 'Time limit exceeded'
```

```
Time to run with size 3000 = 0.3487 seconds
```

2. Parzen Window Classifier implementation (2 Points)

The Parzen Window Classifier prediction model can be written as:

$$h(\mathbf{x}) = \text{sign}(g(\mathbf{x})) = \text{sign}\left(\sum_{i=1}^{n} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}) + b\right),$$

with:

- $g : \mathbb{R}^d \to \mathbb{R}$ being the **decision function**
- $b \in \mathbb{R}$ being the **bias term** defined as:

$$b = \frac{1}{2n_-^2} \sum_{i,j \in I^-} \kappa(\mathbf{x}_i, \mathbf{x}_j) - \frac{1}{2n_+^2} \sum_{i,j \in I^+} \kappa(\mathbf{x}_i, \mathbf{x}_j),$$

- α_i's $\in \mathbb{R}$ being the **dual variables** for all training examples $\mathbf{x}_i$ defined as:

$$\alpha_i = \begin{cases} \frac{1}{n_+} & \text{if } y_i = +1 \\ -\frac{1}{n_-} & \text{if } y_i = -1 \end{cases}.$$

We denote the number of positive / negative training examples as n_+ / n_-, and $n = n_+ + n_-$, and I^+ / I^- are the indices of the positive / negative training examples.

Below you find the class-template for the Parzen Window Classifier. It's functionality is split into three parts:

1. Intialization of Classifier Object using init()

A Parzen Window Classifier instance can be created using its constructor and the kernel to be used can be specified, e.g.:

```
est = ParzenWindowClassifier(kernel="gaussian").
```

2. Model Training using fit()

This function takes as input the features of the training examples $\mathbf{X}_{train}$ and their corresponding labels $\mathbf{y}_{train} \in \{-1, 1\}^{n_{train}}$ and estimates the α_i's and b. The necessary kernel values between the training examples, i.e. $\kappa(\mathbf{x}_i, \mathbf{x}_j)$ are calculated during the fitting process.

```
est.fit(X_train, y_train)
```

3. Prediction for new Examples using predict() and decision_function()

When the model parameters, i.e. b and α_is, are fitted, than we can make predictions for a new example $\mathbf{x}$ using the function $h(\mathbf{x})$.

```
y_test_pred = est.predict(X_test)
```

Task: Implement the missing code parts of `fit()` , `decision_function()` and `predict()` . Make use of the provided formulas (see above).

Hint: The NumPy function `np.sum` can be used to sum over the elements of a matrix.

In [6]:

```
class ParzenWindowClassifier(BaseEstimator, ClassifierMixin):
    def __init__(self, kernel="gaussian", sigma=None):
        """
        Parzen Window Classifier

        :param kernel: string, specifying which kernel to use. Can be 'gaussian' or 'li
near'.
        :param sigma: scalar, gaussian kernel parameter, can be None if the linear kern
el is used.
        """
        # Parzen Window Classifier model parameter
        self.b = None  # bias term
        self.alphas = None  # dual variables

        # Training data needed for the prediction phase
        self.X_train = None

        # Set up kernel function
        self.kernel = kernel
        self.sigma = sigma

    def fit(self, X_train, y_train):
        """
        Fit a Parzen Window Classifier using training data

        :param X_train: array-like, shape=(n_samples, n_features), feature-matrix
        :param y_train: array-like, shape=(n_samples,) or (n_samples, 1), label vector
        """
        # Calculate the specified kernel
        self.X_train = X_train
        KX_train = self._get_kernel(self.X_train)

        # Get indices of positive and negative examples: I_n, I_p
        I_n = [i for i, y in enumerate(y_train) if y == -1 ]
        I_p = [i for i, y in enumerate(y_train) if y == 1 ]

        # Count the number of postitive and negative examples: n_n, n_p
        n_n = len(I_n)
        n_p = len(I_p)

        # Calcualte the bias term: self.b
        self.b = 1/(2*n_n**2) * np.sum(KX_train[I_n][:, I_n]) - 1/(2*n_p**2) * np.sum(K
X_train[I_p][:, I_p])

        # Calculate alpha_i's: self.alpha
        self.alphas = np.zeros((n_n + n_p, 1))
        for i in I_n:
            self.alphas[i] = -1/n_n
        for i in I_p:
            self.alphas[i] = 1/n_p

    def decision_function(self, X):
        """
        Calculate decision function:
            g(x) = sum_i a_i k(x_i, x) + b

        :param X: array-like, shape=(n_samples_test, n_features), feature-matrix of new
```

```
data.
        :return: array-like, shape=(n_samples_test,), decision function value g(x) for
 all new data points
        """
        if self.alphas is None or self.b is None or self.X_train is None:
            raise RuntimeError("Call fit-function first.")

        # Calculate the specified kernel between the training and test examples
        KX_test_train = self._get_kernel(X, self.X_train)

        # Calculate the value of the decision function for each test example
        #print("alphas: ", self.alphas.shape)
        #print("Data: ", KX_test_train.shape)
        #print("b: ", self.b.shape)
        g_X = KX_test_train @ self.alphas + self.b

        return g_X.flatten()  # output a one-dimensional vector

    def predict(self, X):
        """
        Predict labels using Parzen Window Classifier:
            h(x) = sign(g(x)), with g(x) being the decision function

        :param X: array-like, shape=(n_samples_test, n_features), feature-matrix of new
data.
        :return: array-like, shape=(n_samples_test,), predicted labels {-1, 1} for all
 new data points
        """
        if self.alphas is None or self.b is None or self.X_train is None:
            raise RuntimeError("Call fit-function first.")

        # Calculate prediction h(x) = sign(g(x))
        h_X = np.sign(self.decision_function(X))

        return h_X

    def _get_kernel(self, X, Y=None):
        """
        Calcualte kernel matrix using specified kernel-function and parameters.

        :param X: array-like, shape=(n_samples_A, n_features), feature-matrix of set A
        :param Y: array-like, shape=(n_samples_B, n_features), feature-matrix of set B
 or None, than Y = X
        :return: array-like, shape=(n_samples_A, n_samples_B), kernel matrix
        """
        if self.kernel == "gaussian":
            return gaussian_kernel(X, Y, self.sigma)
        elif self.kernel == "linear":
            return linear_kernel(X, Y)
        else:
            raise ValueError("Invalid kernel chosen.")
```

In [7]:

```
X, y = make_blobs(n_samples=50, centers=[[1, 1], [1.5, 1.5]], cluster_std=[0.1, 0.1],
                  random_state=80)
y[y==0] = -1

test_est = ParzenWindowClassifier(kernel="linear")
test_est.fit(X, y)

# Test correct shape of self.b and self.alphas
assert(np.isscalar(test_est.b))
np.testing.assert_equal(test_est.alphas.shape, (50, 1))

# Test correct shape of the predictions
X_test = np.array([[1, 1], [1.5, 1.5], [1, 0], [2, 3]])

# Validate predictions
np.testing.assert_equal(test_est.decision_function(X_test).shape, (4,))

np.testing.assert_equal(test_est.predict(X_test).shape, (4,))
np.testing.assert_equal(test_est.predict(X_test), np.array([-1, 1, -1, 1]))

# Validate score
np.testing.assert_equal(test_est.score(X, y), 1.0)
```

3. Application of the Parzen Window Classifier

It is time to apply your Parzen Window Classifier to some datasets. For that you are given two synthetic datasets $\mathbf{X}$. Each is splitted into a training and test subset: $\mathbf{X}_{train}$ (75%) and $\mathbf{X}_{test}$ (25%).

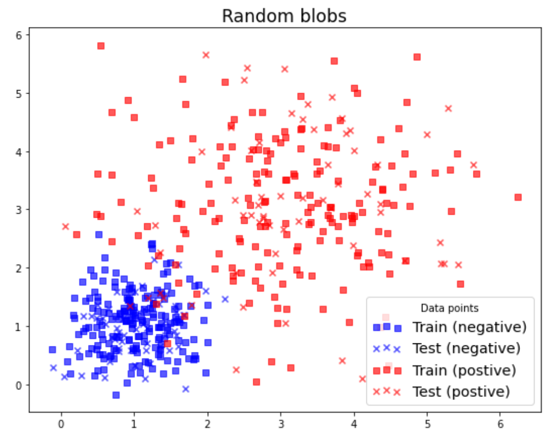
In [8]:

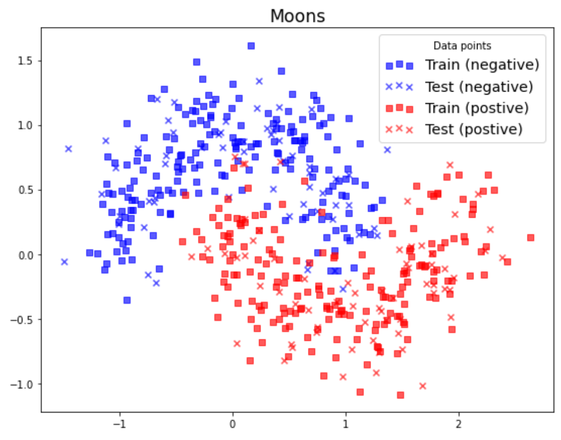
```
# Create synthetic data (Please do not change the random_state!)
X_blobs, y_blobs = make_blobs(n_samples=500, centers=[[1, 1], [3, 3]], cluster_std=[0.5
, 1.15],
                              random_state=80)
X_moons, y_moons = make_moons(n_samples=500, noise=0.25, random_state=797)

# Make labels being {-1, 1}
y_blobs[y_blobs==0] = -1
y_moons[y_moons==0] = -1

# Split data
X_blobs_train, X_blobs_test, y_blobs_train, y_blobs_test = train_test_split(
    X_blobs, y_blobs, random_state=319)
X_moons_train, X_moons_test, y_moons_train, y_moons_test = train_test_split(
    X_moons, y_moons, random_state=747)
```

We can plot the datasets to get an impression what we are dealing with:

In [9]:

```
# Plot datasets
fig, axrr = plt.subplots(1, 2, figsize=(20, 7))

# Blobs
for l_str, l_num, col in [("negative", -1, "blue"), ("postive", 1, "red")]:
    axrr[0].scatter(
        X_blobs_train[y_blobs_train==l_num, 0], X_blobs_train[y_blobs_train==l_num, 1],
        c=col, alpha=0.65, label="Train (%s)" % l_str, marker="s")

    axrr[0].scatter(
        X_blobs_test[y_blobs_test==l_num, 0], X_blobs_test[y_blobs_test==l_num, 1],
        c=col, alpha=0.65, label="Test (%s)" % l_str, marker="x")

# Blobs
for l_str, l_num, col in [("negative", -1, "blue"), ("postive", 1, "red")]:
    axrr[1].scatter(
        X_moons_train[y_moons_train==l_num, 0], X_moons_train[y_moons_train==l_num, 1],
        c=col, alpha=0.65, label="Train (%s)" % l_str, marker="s")

    axrr[1].scatter(
        X_moons_test[y_moons_test==l_num, 0], X_moons_test[y_moons_test==l_num, 1],
        c=col, alpha=0.65, label="Test (%s)" % l_str, marker="x")


axrr[0].set_title("Random blobs", fontsize="xx-large")
axrr[0].legend(title="Data points", fontsize="x-large", scatterpoints=3)

axrr[1].set_title("Moons", fontsize="xx-large")
axrr[1].legend(title="Data points", fontsize="x-large", scatterpoints=3)

plt.show()
```





A. Implement the hyper parameter optimization (1 point)

Train (fit) your Parzen Window Classifier with Gaussian kernel on the training examples, i.e. `X_blobs_train` and `X_moons_train` . To find the optimal Gaussian bandwidth parameter σ we search a grid of different parameter values and score each one using CV.

Task: Implement the missing code parts of the `hyper_parameter_search_using_cv` function.

The function gets in a set of training examples and a grid of different parameters, e.g. σ's, calculates an average validation set score for all of them using cross-validation. Subsequently, a model using all the training data ist used, to train a model with the best set of parameters.

Hints: - Make use of the Python tutorial (fetch on JupyterHub), if you want to see the pseudo-code of the parameter search. - Read the documentation of the sklearn [`KFold` function](https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.KFold.html#sklearn.model_selection.KFold). - You can calculate the performance score using `est.score(...)` . Read also: https://scikit-learn.org/stable/modules/generated/sklearn.base.ClassifierMixin.html#sklearn.base.ClassifierMixin.score

In [10]:

```
def hyper_parameter_search_using_cv(estimator, X, y, param_grid, n_cv_folds=5,
                                    random_state=None):
    """
    Function calculating the estimator score for a grid of hyper parameters.

    :param estimator: object, subclass of RegressorMixin or ClassifierMixin and BaseEst
imator
    :param X: array-like, shape=(n_samples, n_features), feature-matrix used for traini
ng
    :param y: array-like, shape=(n_samples,) or (n_samples, 1), label vector used for t
raining
    :param param_grid: dictionary,
        keys: different parameter names
        values: grid-values for each parameter
    :param n_cv_folds: scalar, a KFold cross-validation is performed where the number o
f splits is equal the scalar.
    :param random_state: scalar, RandomState instance or None, optional, default=None
        If int, random_state is the seed used by the random number generator;
        If RandomState instance, random_state is the random number generator;
        If None, the random number generator is the RandomState instance used
        by `np.random`.

    :return: tuple = (
            best estimator,
            param grid as list and corresponding evaluation scores,
            score of best parameter
            best parameter
        )
    """
    # Get an iterator over all parameters
    param_grid_iter = ParameterGrid(param_grid)

    # Create cross-validation object
    cv = KFold(n_splits=n_cv_folds, shuffle=True, random_state=random_state)

    # Store the valdidation set performance scores for all folds and parameters
    perf_scores = np.zeros((cv.get_n_splits(), len(param_grid_iter)))

    for fold, (train_set, val_set) in enumerate(cv.split(X, y)):
        # Separate training and validation set from X and y,
        #  i.e. X_train, X_val, y_train and y_val
        X_train =  X[train_set]
        X_val =  X[val_set]
        y_train =  y[train_set]
        y_val =  y[val_set]

        for idx, param in enumerate(param_grid_iter):
            # Clone the estimator object to get an un-initialized object
            est = clone(estimator)

            # Set model parameters
            est.set_params(**param)

            # Fit the model using training set
            est.fit(X_train, y_train)

            # Calculate the perf. score on validation set for current fold and paramete
```

```
r index
            perf_scores[fold, idx] = est.score(X_val, y_val)

    # Find best performing hyper-parameter

    # Average the perf. scores for each parameter across each fold
    avg_perf_scores = np.mean(perf_scores, axis = 0)

    idx_best = np.argmax(avg_perf_scores)
    best_perf_score = avg_perf_scores[idx_best]
    best_param = param_grid_iter[idx_best]

    # Fit model using all data with the best parameters
    est = clone(estimator)
    est.set_params(**best_param)
    est.fit(X, y)

    return (est, {"params": list(param_grid_iter), "scores": avg_perf_scores},
            best_perf_score, best_param)
```

In [11]:

```
X, y = make_blobs(n_samples=100, centers=[[1, 1], [1.5, 1.5]], cluster_std=[0.2, 0.75],
                  random_state=100)
y[y==0] = -1

_param_grid = {"sigma": [0.05, 0.1, 0.5, 1.]}
_est, _param_scores, _best_score, _best_param = hyper_parameter_search_using_cv(
    ParzenWindowClassifier(kernel="gaussian"), X, y, _param_grid, random_state=100)

np.testing.assert_equal(_param_scores["scores"].shape, (len(_param_grid["sigma"]),))
np.testing.assert_allclose(_param_scores["scores"], np.array([0.85, 0.9, 0.9, 0.83]))
np.testing.assert_equal(_best_param, {"sigma": 0.1})
np.testing.assert_allclose(_best_score, 0.9)
assert(isinstance(_est, ParzenWindowClassifier))
```

B. Plot validation score for different hyper parameters

With the hyper parameter optimization function at hand, we find the best σ parameter for the two synthetic datasets and also inspect the average validation error for different values of σ.

First let us the parameter grid for the Gaussian kernel bandwidth parameter σ:

In [12]:

```
param_grid = {"sigma": [0.01, 0.05, 0.1, 0.5, 1, 5, 10, 50]}
```

Now we run the `hyper_parameter_search_using_cv` function for `X_blobs_train` and `X_blobs_test` :

In [13]:

```
est_blobs, scores_blobs, best_score_blobs, best_param_blobs = hyper_parameter_search_us
ing_cv(
    ParzenWindowClassifier(kernel="gaussian"), X_blobs_train, y_blobs_train, param_grid
,
    random_state=737)

print("[Blobs] Best average validation score", best_score_blobs)
print("[Blobs] Best parameter", best_param_blobs)

est_moons, scores_moons, best_score_moons, best_param_moons = hyper_parameter_search_us
ing_cv(
    ParzenWindowClassifier(kernel="gaussian"), X_moons_train, y_moons_train, param_grid
,
    random_state=747)

print("[Moons] Best average validation score", best_score_moons)
print("[Moons] Best parameter", best_param_moons)
```

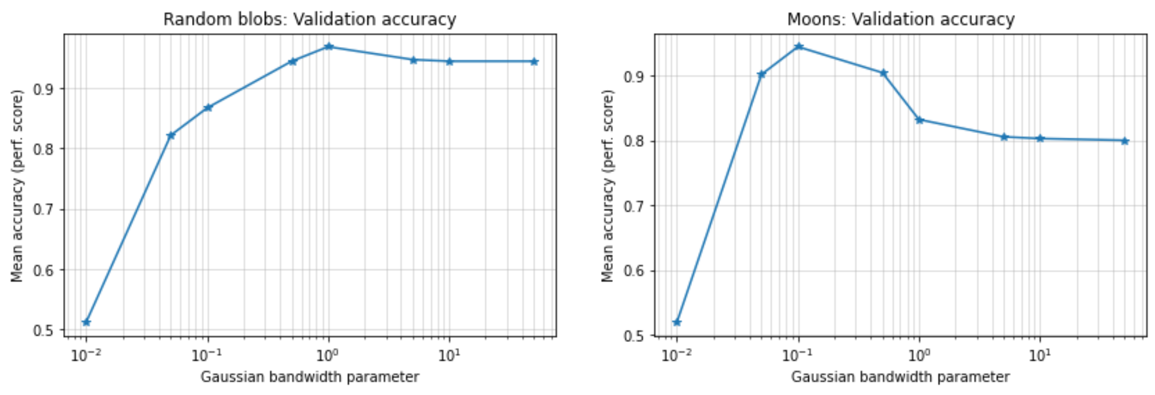
```
[Blobs] Best average validation score 0.968
[Blobs] Best parameter {'sigma': 1}
[Moons] Best average validation score 0.944
[Moons] Best parameter {'sigma': 0.1}
```

Plot validation score for the different parameter values.

Hint: Both curves should have a single maxima, if you did not change any random seeds, i.e. `random_state` values, or data generation parameters. Otherwise, it could be that multiple σ's are equally good. However, overall it should be a function with single maxima (maybe a region).

In [14]:

```
fig, axrr = plt.subplots(1, 2, figsize=(14, 4), sharex="row")

axrr[0].plot(param_grid["sigma"], scores_blobs["scores"], '*-')
axrr[0].set_xscale("log")
axrr[0].grid(True, which="both", ls="-", alpha=0.5)
axrr[0].set_title("Random blobs: Validation accuracy")
axrr[0].set_xlabel("Gaussian bandwidth parameter")
axrr[0].set_ylabel("Mean accuracy (perf. score)")

axrr[1].plot(param_grid["sigma"], scores_moons["scores"], '*-')
axrr[1].set_xscale("log")
axrr[1].grid(True, which="both", ls="-", alpha=0.5)
axrr[1].set_title("Moons: Validation accuracy")
axrr[1].set_xlabel("Gaussian bandwidth parameter")
axrr[1].set_ylabel("Mean accuracy (perf. score)")

plt.show()
```



The hyper-parameter optimization was done only using the training data. We now can apply the best model (with the optimal σ parameter) to the training data. We should see a similar performance as for the validation set:

In [15]:

```
print("[Blobs] Score on test set", est_blobs.score(X_blobs_test, y_blobs_test))
print("[Moons] Score on test set", est_moons.score(X_moons_test, y_moons_test))
```

```
[Blobs] Score on test set 0.936
[Moons] Score on test set 0.912
```

4. Model visualization: Non-linear vs. Linear (no points)

Bonus task: Here we inspect the decision function and how it separates the two classes in the feature space. For that we will evaluate $g(\mathbf{x})$ for $\mathbf{x}$'s on a regular grid. 1. Set up interval to plot decision function, e.g. min. and max. value of our synthetic datasets. 2. Create grid-points $\mathbf{x}$ covering the intervall. 3. Evaluate $z = g(\mathbf{x})$ for all points. 4. Plot the z's for different points and color them according to their sign.

In [16]:

```
def get_gridpoints(X):
    """
    :param X: array-like, shape=(n_samples, d), datset feature matrix

    :return: array-like, shape=(n_grid_samples, d), feature vectors on a regular grid i
n the feature space
    """
    x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
    y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1

    xx, yy = np.meshgrid(np.arange(x_min, x_max, 0.1),
                         np.arange(y_min, y_max, 0.1))

    return xx, yy

def get_color_normalizer(Z, n_colors=256, n_point=10):
    bounds = np.append(np.linspace(np.min(Z), 0, n_point)[:-1], np.linspace(0, np.max(Z
), n_point))  # do not add zero twice
    return colors.BoundaryNorm(boundaries=bounds, ncolors=n_colors)
```

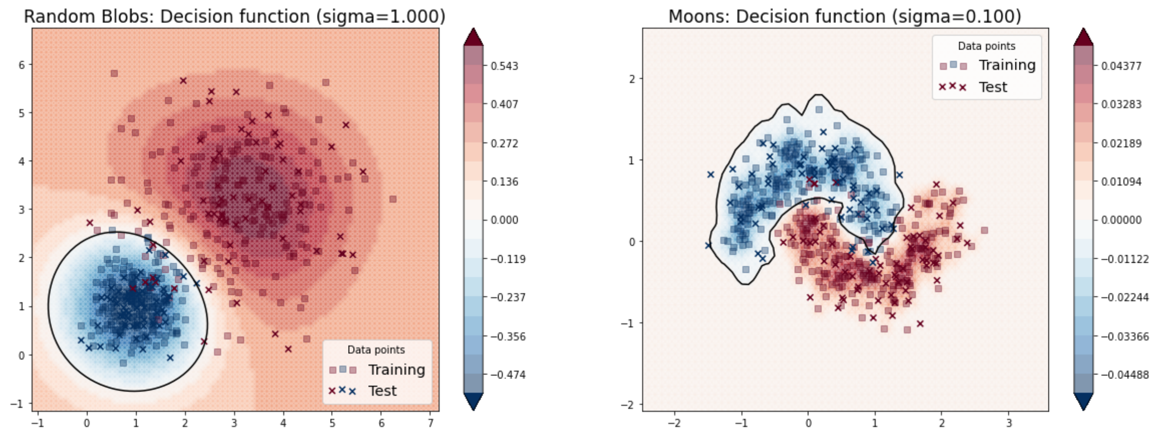
Decision Function for Gaussian Kernel (Model of previous tasks)

In [17]:

```
XX_blobs_grid, YY_blobs_grid = get_gridpoints(X_blobs)
Z_blobs_grid = est_blobs.decision_function(np.c_[XX_blobs_grid.ravel(), YY_blobs_grid.r
avel()])
Z_blobs_grid = Z_blobs_grid.reshape(XX_blobs_grid.shape)

XX_moons_grid, YY_moons_grid = get_gridpoints(X_moons)
Z_moons_grid = est_moons.decision_function(np.c_[XX_moons_grid.ravel(), YY_moons_grid.r
avel()])
Z_moons_grid = Z_moons_grid.reshape(XX_moons_grid.shape)
```

In [18]:

```
fig, axrr = plt.subplots(1, 2, figsize=(20, 7))

# plot contours, levels, ...
pcm = axrr[0].pcolormesh(XX_blobs_grid, YY_blobs_grid, Z_blobs_grid, alpha=0.5, shading="gouraud",
                         norm=get_color_normalizer(Z_blobs_grid))
fig.colorbar(pcm, ax=axrr[0], extend="both", orientation="vertical")
axrr[0].contour(XX_blobs_grid, YY_blobs_grid, Z_blobs_grid, colors=['k'], linestyles=['-'], levels=[0])

# plot points
axrr[0].scatter(X_blobs_train[:, 0], X_blobs_train[:, 1], c=y_blobs_train, marker="s", alpha=0.35)
axrr[0].scatter(X_blobs_test[:, 0], X_blobs_test[:, 1], c=y_blobs_test, marker="x")

# plot labels, titles, ...
axrr[0].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3)
axrr[0].set_title("Random Blobs: Decision function (sigma=%.3f)" % best_param_blobs["sigma"],
                  fontsize="xx-large")

pcm = axrr[1].pcolormesh(XX_moons_grid, YY_moons_grid, Z_moons_grid, alpha=0.5, shading="gouraud",
                         norm=get_color_normalizer(Z_moons_grid))
fig.colorbar(pcm, ax=axrr[1], extend="both", orientation="vertical")
axrr[1].scatter(X_moons_train[:, 0], X_moons_train[:, 1], c=y_moons_train, marker="s", alpha=0.35)
axrr[1].scatter(X_moons_test[:, 0], X_moons_test[:, 1], c=y_moons_test, marker="x")
axrr[1].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3)
axrr[1].set_title("Moons: Decision function (sigma=%.3f)" % best_param_moons["sigma"],
                  fontsize="xx-large")
axrr[1].contour(XX_moons_grid, YY_moons_grid, Z_moons_grid, colors=['k'], linestyles=['-'], levels=[0])

plt.show()
```



Decision Function for Linear Kernel

We have seen that the Gaussian kernel leads to a non-linear decision boundary, i.e. $g(\mathbf{x}) = 0$ (black line in plots). Now we take a look on the linear Parzen Window Classifier, buy using a linear kernel.

In [19]:

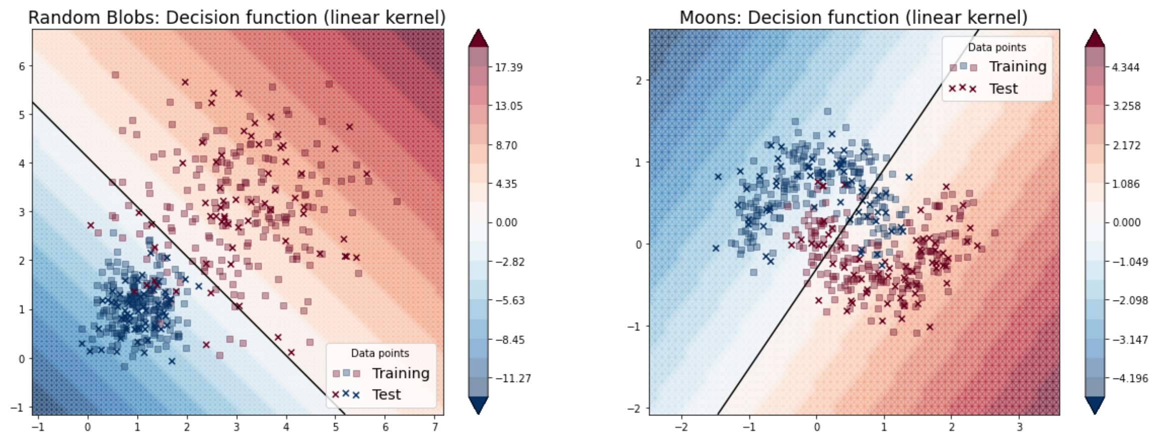
```
est_blobs = ParzenWindowClassifier(kernel="linear")
est_blobs.fit(X_blobs_train, y_blobs_train)

est_moons = ParzenWindowClassifier(kernel="linear")
est_moons.fit(X_moons_train, y_moons_train)
```

In [20]:

```
XX_blobs_grid, YY_blobs_grid = get_gridpoints(X_blobs)
Z_blobs_grid = est_blobs.decision_function(np.c_[XX_blobs_grid.ravel(), YY_blobs_grid.r
avel()])
Z_blobs_grid = Z_blobs_grid.reshape(XX_blobs_grid.shape)

XX_moons_grid, YY_moons_grid = get_gridpoints(X_moons)
Z_moons_grid = est_moons.decision_function(np.c_[XX_moons_grid.ravel(), YY_moons_grid.r
avel()])
Z_moons_grid = Z_moons_grid.reshape(XX_moons_grid.shape)
```

In [21]:

```
fig, axrr = plt.subplots(1, 2, figsize=(20, 7))

# plot contours, levels, ...
pcm = axrr[0].pcolormesh(XX_blobs_grid, YY_blobs_grid, Z_blobs_grid, alpha=0.5, shading="gouraud",
                         norm=get_color_normalizer(Z_blobs_grid))
fig.colorbar(pcm, ax=axrr[0], extend="both", orientation="vertical")
axrr[0].contour(XX_blobs_grid, YY_blobs_grid, Z_blobs_grid, colors=['k'], linestyles=['-'], levels=[0])

# plot points
axrr[0].scatter(X_blobs_train[:, 0], X_blobs_train[:, 1], c=y_blobs_train, marker="s", alpha=0.35)
axrr[0].scatter(X_blobs_test[:, 0], X_blobs_test[:, 1], c=y_blobs_test, marker="x")

# plot labels, titles, ...
axrr[0].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3)
axrr[0].set_title("Random Blobs: Decision function (linear kernel)", fontsize="xx-large")

pcm = axrr[1].pcolormesh(XX_moons_grid, YY_moons_grid, Z_moons_grid, alpha=0.5, shading="gouraud",
                         norm=get_color_normalizer(Z_moons_grid))
fig.colorbar(pcm, ax=axrr[1], extend="both", orientation="vertical")
axrr[1].scatter(X_moons_train[:, 0], X_moons_train[:, 1], c=y_moons_train, marker="s", alpha=0.35)
axrr[1].scatter(X_moons_test[:, 0], X_moons_test[:, 1], c=y_moons_test, marker="x")
axrr[1].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3)
axrr[1].set_title("Moons: Decision function (linear kernel)", fontsize="xx-large")
axrr[1].contour(XX_moons_grid, YY_moons_grid, Z_moons_grid, colors=['k'], linestyles=['-'], levels=[0])

plt.show()
```


Random Blobs: Decision function (linear kernel)
Data points
Training
Test
Moons: Decision function (linear kernel)