Solutions to Assignment 1 of CS-E4830 Kernel Methods in Machine Learning 2021

Pen and paper exercise

Question 1 (2 points): Recall from the Lecture 1, the general form for the polynomial kernel

$$K(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^m = (\mathbf{x}^T \mathbf{y} + c)^m$$

where $c \geq 0$, m is a positive integer and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.

- Prove that $K(\mathbf{x}, \mathbf{y})$ is a valid kernel

Solution

- Given $K(\mathbf{x}, \mathbf{y}) = (\langle \mathbf{x}, \mathbf{y} \rangle + c)^m$ given that $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$.
- Using Binomial Theorem : $(\langle \mathbf{x}, \mathbf{y} \rangle)^m$ can be expanded as follows:

$$\binom{m}{0}(\langle \mathbf{x}, \mathbf{y} \rangle)^m c^0 + \binom{m}{1}(\langle \mathbf{x}, \mathbf{y} \rangle)^{m-1} c^1 + \ldots + \binom{m}{m}(\langle \mathbf{x}, \mathbf{y} \rangle)^0 c^m$$

- Now, $\langle \mathbf{x}, \mathbf{y} \rangle$ is an inner product in $\mathbb{R}^d$, hence it is a kernel.
- Since product of kernels is a kernel, therefore $(\langle \mathbf{x}, \mathbf{y} \rangle)^2$, and $(\langle \mathbf{x}, \mathbf{y} \rangle)^3$ and so on are also kernels
- Furthermore, multiplying a kernel by a positive number is also a kernel
- Therefore, all the terms (except the last term which is a constant), and hence their sum is a kernel. Call it $K_s(\mathbf{x}, \mathbf{y})$, and its corresponding feature map be $\phi(.)$ such that $K_s(\mathbf{x}, \mathbf{y}) = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle$
- Call the last term α, therefore we have $K(\mathbf{x}, \mathbf{y}) = K_s(\mathbf{x}, \mathbf{y}) + \alpha = \langle \phi(\mathbf{x}), \phi(\mathbf{y}) \rangle + \alpha$
- Therefore, $K(.,.)$ can be expressed as an inner product with the following feature map $\begin{bmatrix} \phi(\mathbf{x}) \\ \sqrt{\alpha} \end{bmatrix}$.
- Hence $K(.,.)$ is a kernel.

Question 2 (4 points): Recall from lecture 2, in the context of binary classification, the Parzen window classifier assigns a test instance x based on the distance to the centroids in the following way:

$$h(x) = \begin{cases} +1 & \text{if} \quad \|\phi(x) - c_-\|^2 > \|\phi(x) - c_+\|^2 \\ -1 & \text{otherwise.} \end{cases}$$

where c_- and c_+ represent the centroids in the feature space of the negative and positive classes respectively. Show by deriving appropriate expressions for α_i and b that the above decision function can be written in the following form $h(x) = \text{sgn}(\sum_{i=1}^{n} \alpha_i k(x, x_i) + b)$ such that $k(x, x_i) = \langle \phi(x), \phi(x_i) \rangle$. Here sgn(.) represents the sign function, and n is the total number of training samples.

Solution

- We can rewrite $h(x) = \text{sgn}(\|\phi(x) - c_-\|^2 - \|\phi(x) - c_+\|^2)$
- Using $\|x\|^2 = \langle x, x \rangle$ we have $h(x) = \text{sgn}(\langle \phi(x) - c_-, \phi(x) - c_- \rangle - \langle \phi(x) - c_+, \phi(x) - c_+ \rangle)$
- Now expanding the terms inside the sgn(.) using properties $\langle x, y + z \rangle = \langle x, y \rangle + \langle x, z \rangle$ we have

  $$\langle \phi(x) - c_-, \phi(x) - c_- \rangle - \langle \phi(x) - c_+, \phi(x) - c_+ \rangle = 2\langle \phi(x), c_+ \rangle - 2\langle \phi(x), c_- \rangle + \langle c_-, c_- \rangle - \langle c_+, c_+ \rangle$$

- As sgn(.) is unaffected by a positive multiple we can write

  $$h(x) = \text{sgn}(\langle \phi(x), c_+ \rangle - \langle \phi(x), c_- \rangle + 0.5\langle c_-, c_- \rangle - 0.5\langle c_+, c_+ \rangle)$$

- Now using the definitions of c_+ and c_- we can expand each term using properties of inner products as follows

$$\begin{aligned} \langle \phi(x), c_+ \rangle &= \left\langle \phi(x), \frac{1}{m_+} \sum_{i \in \mathcal{I}^+} \phi(x_i) \right\rangle \\ &= \frac{1}{m_+} \left\langle \phi(x), \sum_{i \in \mathcal{I}^+} \phi(x_i) \right\rangle && \because \langle ax, y \rangle = a\langle x, y \rangle \\ &= \frac{1}{m_+} \sum_{i \in \mathcal{I}^+} \langle \phi(x), \phi(x_i) \rangle && \because \langle x, y + z \rangle = \langle x, y \rangle + \langle y, z \rangle \\ &= \frac{1}{m_+} \sum_{i \in \mathcal{I}^+} k(x, x_i) \end{aligned}$$

Similarly $\langle \phi(x), c_- \rangle = \frac{1}{m_-} \sum_{i \in \mathcal{I}^-} k(x, x_i)$

- A similar process for $\langle c_-, c_- \rangle$

$$\begin{aligned}\langle c_-, c_- \rangle &= \left\langle \frac{1}{m_-} \sum_{i \in \mathcal{I}^-} \phi(x_i), \frac{1}{m^-} \sum_{j \in \mathcal{I}^-} \phi(x_j) \right\rangle \\ &= \frac{1}{m_-^2} \left\langle \sum_{i \in \mathcal{I}^-} \phi(x_i), \sum_{j \in \mathcal{I}^-} \phi(x_j) \right\rangle \\ &= \frac{1}{m_-^2} \sum_{i \in \mathcal{I}^-} \sum_{j \in \mathcal{I}^-} \langle \phi(x_i), \phi(x_j) \rangle \\ &= \frac{1}{m_-^2} \sum_{i,j \in \mathcal{I}^-} k(x_i, x_j)\end{aligned}$$

  Similarly $\langle c_+, c_+ \rangle = \frac{1}{m_+^2} \sum_{i,j \in \mathcal{I}^+} k(x_i, x_j)$

- We can now take $b = 0.5(\langle c_-, c_- \rangle - \langle c_+, c_+ \rangle)$, therefore

$$b = \frac{1}{2m_-^2} \sum_{i,j \in \mathcal{I}^-} k(x_i, x_j) - \frac{1}{2m_+^2} \sum_{i,j \in \mathcal{I}^+} k(x_i, x_j)$$

- Now combining all previous results we have

$$h(x) = \operatorname{sgn}\left(\frac{1}{m_+} \sum_{i \in \mathcal{I}^+} k(x, x_i) - \frac{1}{m_-} \sum_{i \in \mathcal{I}^-} k(x, x_i) + b \right)$$

- As $\mathcal{I} = \mathcal{I}^+ \cup \mathcal{I}^-$ and $n = m_+ + m_-$ we can combine the integrals by introducing a coefficient term α_i like

$$h(x) = \operatorname{sgn}\left(\sum_{i=1}^{n} \alpha_i k(x, x_i) + b \right)$$

  Where

$$\begin{cases} \frac{1}{m_+}, & y_i = +1 \\ \frac{-1}{m_-}, & y_i = -1 \end{cases}$$

  Hence derived

Question 3 (3 points): For $x, y \in \mathbb{R}$ check if $K_2(x, y) = \cos(x + y)$ is a valid kernel function.

Solution: Recall from lecture 2 that a kernel function needs to be positive definite. A symmetric function $k : \mathcal{X} \times \mathcal{X} \mapsto \mathbb{R}$ is positive definite if $\forall n \geq 1, \forall (a_1, ..., a_n) \in \mathbb{R}^n, \forall (x_1, ..., x_n) \in \mathcal{X}^n$,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j k(x_i, x_j) \geq 0$$

The above should hold even for a single point, i.e., $a^2 k(x, x) \geq 0$ for all $x \in \mathcal{X}$ and $a \in \mathbb{R}$

Now, take $x = \frac{\pi}{2}$ and $a = 1$. In this case, it is $1^2 \times \cos(\pi/2 + \pi/2) = -1 < 0$. Hence it is not a kernel. Of course, there could be many other counter-examples.

Question 4 (3 points): For $x, y \in \mathcal{X} = (-1, 1)$, prove that $K_3(x, y) = \frac{1}{1-xy}$ is a valid kernel

Solution: Since $x, y \in \mathcal{X} = (-1, 1)$, therefore, $K_3(x, y) = \frac{1}{1-xy} = 1+xy+(xy)^2+(xy)^3+....$ Each of individual terms (apart from 1) is a kernel, either by definition or product of kernels is a kernel property. Hence the sum of kernels is also kernel. The sum of kernel and a constane (the first term 1) is also a kernel as well. Hence $K_3(x, y)$ is a kernel.

Exercise 01

Kernel Methods in Machine Learning (CS-E4830)

Submission deadline: 30.3.2021 at 4pm

Tutorial session: 18.3.2021 at 4:15pm - 6pm

Tasks: 1. [Implement kernel matrix calculation](#task_1) 1. [Linear kernel](#task_1_a) (**2 Point**) 2. [Gaussian kernel](#task_1_b) (**2 Point**) 2. [Implement the Parzen Window Classifier](#task_2) (**3 Point**) 3. [Application of the Parzen Window Classifier](#task_3) 1. [Implement the hyper parameter optimization](#task_3_a) (**3 Point**) 2. [Plot validation score for different hyper parameters](#task_3_b)(**0 Point**)

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

Version: 1.2

Version history:

- 1.0: Initial version
- 1.1: Fix typo: Parzen Window Clf. dual-variables (alpha) had wrong sign in formula. Issue on MyCourses (https://mycourses.aalto.fi/mod/forum/discuss.php?d=128291)
- 1.2: Fix typo: Gaussian kernel doc-string, put brackets around the denominator within exponential function.

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

EMAIL: firstname.lastname@aalto.fi

STUDENT_NUMBER: please_fill_in

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_test_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 (2 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]:
```
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, than Y = X

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

    # YOUR CODE HERE
    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 = 0.0004 seconds
```

B. Gaussian kernel (2 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)

    # YOUR CODE HERE
    K_A_lin_diag = np.sum(X_A * X_A, axis=1)[:, np.newaxis]  # diag(K_X), shape=(n_A, 1)
    K_B_lin_diag = np.sum(X_B * X_B, axis=1)[np.newaxis, :]  # diag(K_Y), shape=(1, n_B)

    K_AB_lin = X_A @ X_B.T

    K_AB = (K_A_lin_diag @ np.ones((1, n_B)) + np.ones((n_A, 1)) @ K_B_lin_diag - 2 * K_AB_lin)  # ||x_i - x_j||^2
    K_AB /= (-2. * sigma**2)
    K_AB = np.exp(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 = 0.4363 seconds
```

2. Parzen Window Classifier implementation (3 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:

- $g : \mathbb{R}^d \rightarrow \mathbb{R}$ 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 'linear'.
        :param sigma: scalar, gaussian kernel parameter, can be None if the linear kernel 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
        # YOUR CODE HERE
        I_n = (y_train == -1)
        I_p = (y_train == 1)

        # Count the number of postitive and negative examples: n_n, n_p
        # YOUR CODE HERE
        n_n = np.sum(I_n)
        n_p = np.sum(I_p)
```

```
        # Calcualte the bias term: self.b
        # YOUR CODE HERE
        b_n = np.sum(KX_train[I_n][:, I_n]) / (2. * n_n ** 2)
        b_p = np.sum(KX_train[I_p][:, I_p]) / (2. * n_p ** 2)
        self.b = b_n - b_p

        # Calculate alpha_i's: self.alpha
        self.alphas = np.zeros((n_n + n_p, 1))
        # YOUR CODE HERE
        self.alphas[I_n] = -1. / n_n
        self.alphas[I_p] = 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 poin
ts
        """
        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
        # YOUR CODE HERE
        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))
        # YOUR CODE HERE
        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)
```

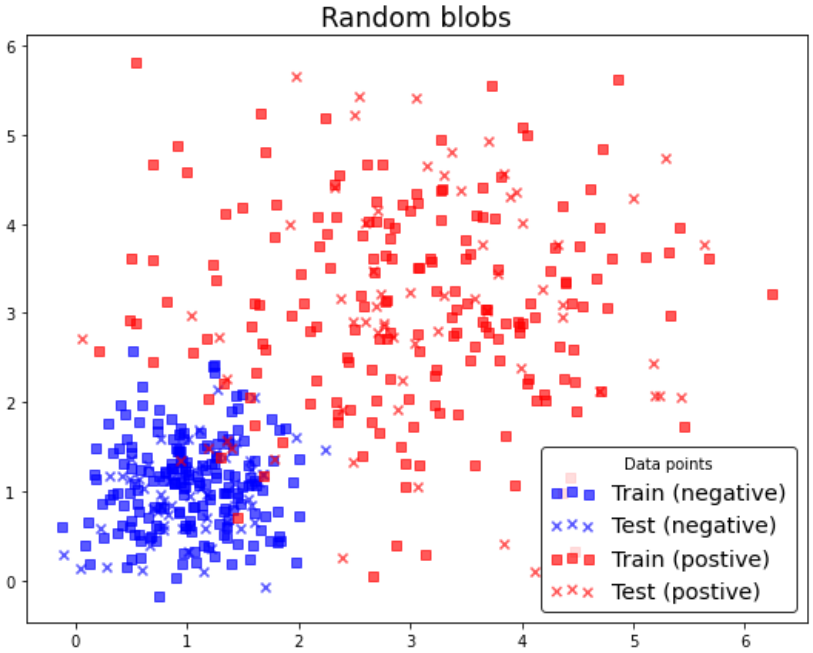
3. Application of the Parzen Window Classifier

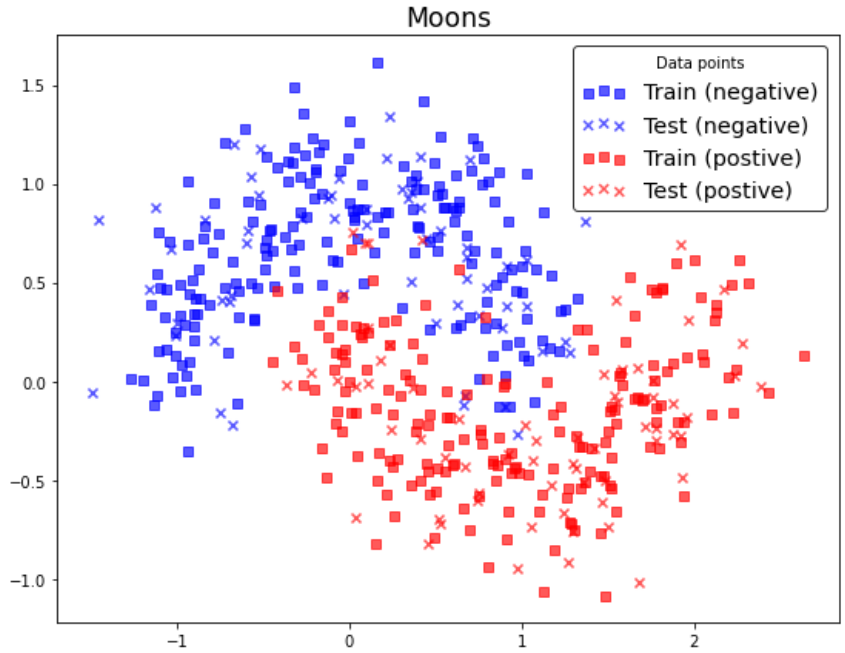
It is time to apply your Parzen Window Classifier to some datasets. For that you are given two synthetic datasets $\mathbf{X}$. Each is splitted into a training and test subset: $\mathbf{X}_{train}$ (75%) and $\mathbf{X}_{test}$ (25%).

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, edgecolor="k")

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

plt.show()
```


Random blobs
Data points
Train (negative)
Test (negative)
Train (postive)
Test (postive)


Moons
Data points
Train (negative)
Test (negative)
Train (postive)
Test (postive)

A. Implement the hyper parameter optimization (3 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 BaseEstimator
    :param X: array-like, shape=(n_samples, n_features), feature-matrix used for training
    :param y: array-like, shape=(n_samples,) or (n_samples, 1), label vector used for training
    :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 of 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, 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
        # YOUR CODE HERE
```

```
            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
                # YOUR CODE HERE
                est.fit(X_train, y_train)

                # Calculate the perf. score on validation set for current fold and parameter index
                # YOUR CODE HERE
                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
    # YOUR CODE HERE
    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)

np.testing.assert_equal(_param_scores["scores"].shape, (len(_param_grid["sigma"]),))
np.testing.assert_allclose(_param_scores["scores"], np.array([0.83, 0.91, 0.89, 0.83]))
np.testing.assert_equal(_best_param, {"sigma": 0.1})
np.testing.assert_allclose(_best_score, 0.91)
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` :

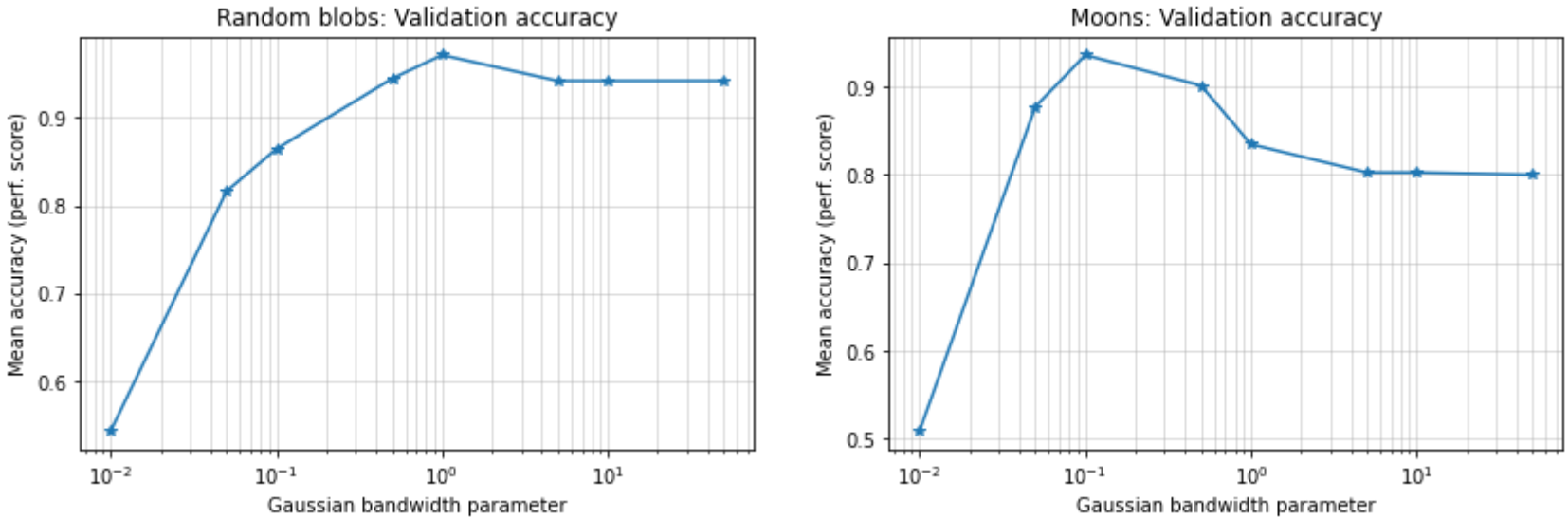
In [13]:
```
est_blobs, scores_blobs, best_score_blobs, best_param_blobs = hyper_parameter_search_using_cv(
    ParzenWindowClassifier(kernel="gaussian"), X_blobs_train, y_blobs_train, param_grid,
    random_state=737)

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_using_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)
```

```
/opt/conda/lib/python3.8/site-packages/sklearn/model_selection/_split.py:293: FutureWarning: Setting a r
andom_state has no effect since shuffle is False. This will raise an error in 0.24. You should leave ran
dom_state to its default (None), or set shuffle=True.
  warnings.warn(

[Blobs] Best average validation score 0.9706666666666667
[Blobs] Best parameter {'sigma': 1}
[Moons] Best average validation score 0.9359999999999999
[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)

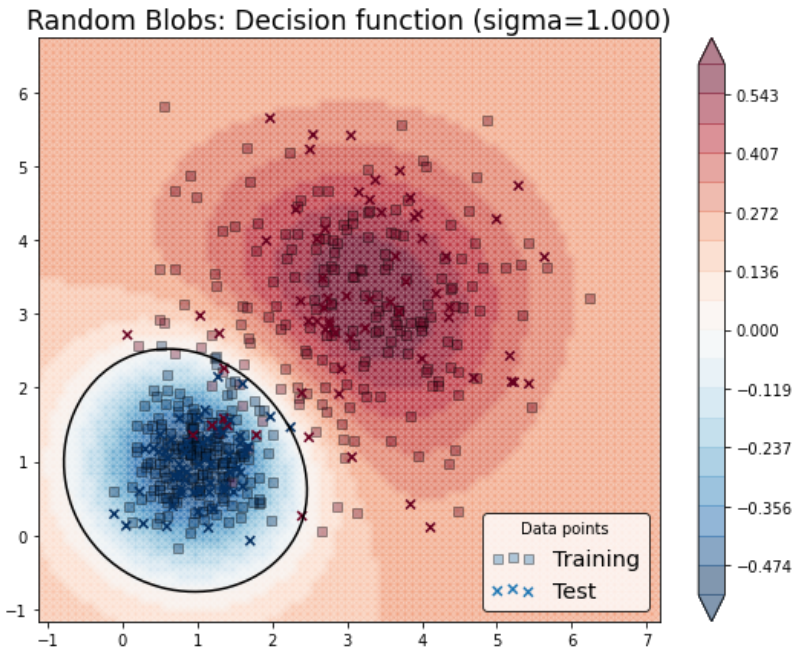
Bonus task: Here we inspect the decision function and how it separates the two classes in the feature space. For that we will evaluate $g(\mathbf{x})$ for $\mathbf{x}$'s on a regular grid. 1. Set up interval to plot decision function, e.g. min. and max. value of our synthetic datasets. 2. Create grid-points $\mathbf{x}$ 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.

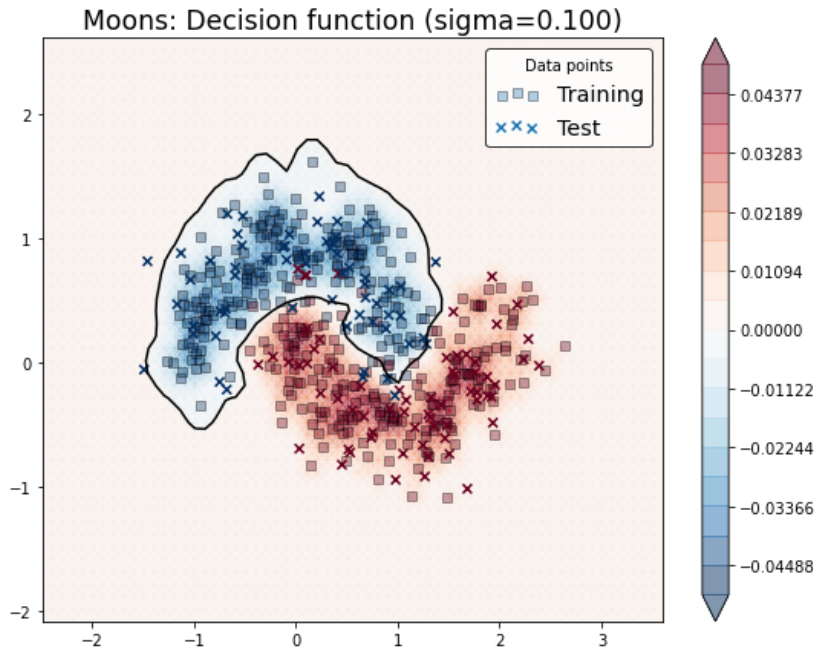
In [16]:
```
def get_gridpoints(X):
    """
    :param X: array-like, shape=(n_samples, d), datset feature matrix

    :return: array-like, shape=(n_grid_samples, d), feature vectors on a regular grid in the feature spa
ce
    """
    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))  # d
o 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.ravel()])
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.ravel()])
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", edgecolors="k", a
lpha=0.35)
axrr[0].scatter(X_blobs_test[:, 0], X_blobs_test[:, 1], c=y_blobs_test, marker="x", edgecolors="k")

# plot labels, titles, ...
axrr[0].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3, edgecolor
="k")
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", edgecolors="k", a
lpha=0.35)
axrr[1].scatter(X_moons_test[:, 0], X_moons_test[:, 1], c=y_moons_test, edgecolors="k", marker="x")
axrr[1].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3, edgecolor
="k")
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()
```





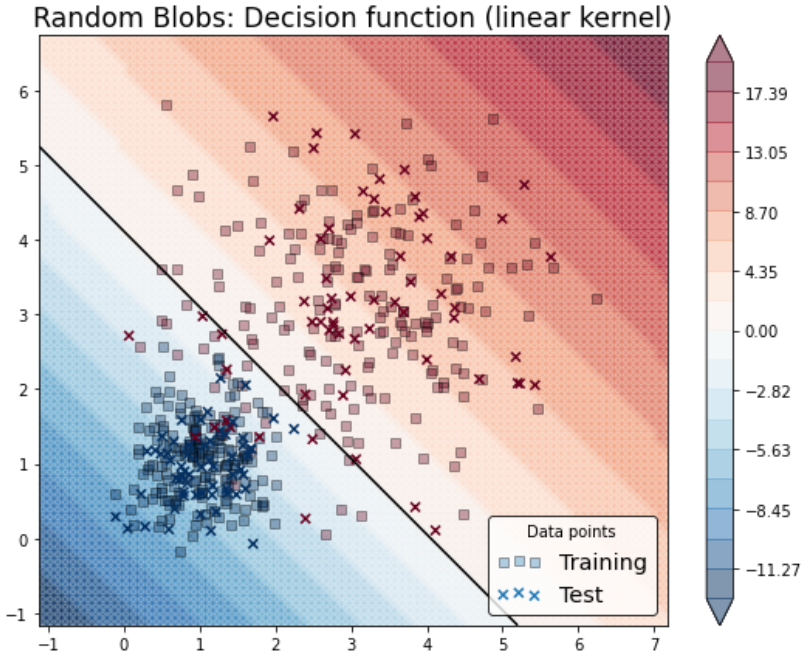
Decision Function for Linear Kernel

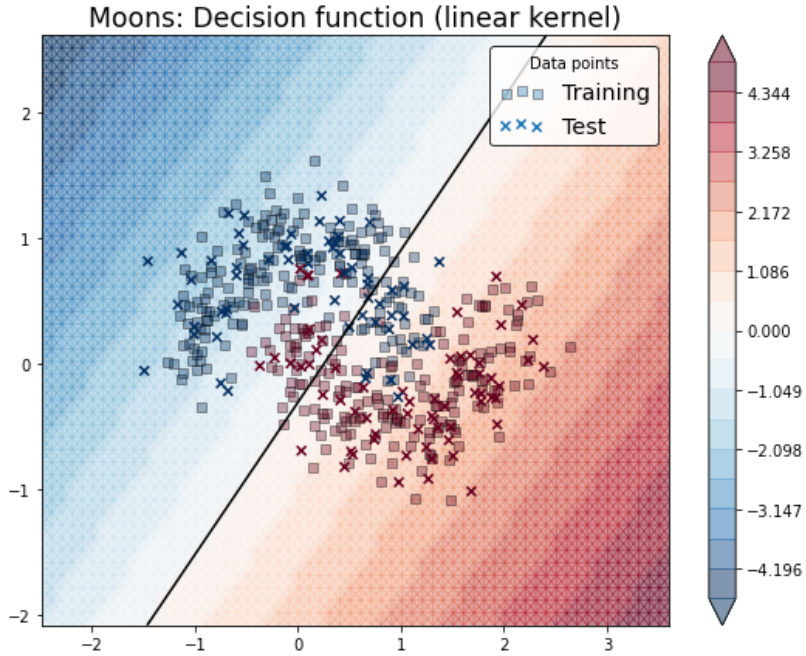
We have seen that the Gaussian kernel leads to a non-linear decision boundary, i.e. $g(\mathbf{x}) = 0$ (black line in plots). Now we take a look on the linear Parzen Window Classifier, buy using a linear kernel.

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.ravel()])
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.ravel()])
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", edgecolors="k", a
lpha=0.35)
axrr[0].scatter(X_blobs_test[:, 0], X_blobs_test[:, 1], c=y_blobs_test, edgecolors="k", marker="x")

# plot labels, titles, ...
axrr[0].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3, edgecolor
="k")
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", edgecolors="k", a
lpha=0.35)
axrr[1].scatter(X_moons_test[:, 0], X_moons_test[:, 1], c=y_moons_test, edgecolors="k", marker="x")
axrr[1].legend(["Training", "Test"], title="Data points", fontsize="x-large", scatterpoints=3, edgecolor
="k")
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
17.39
13.05
8.70
4.35
0.00
−2.82
−5.63
−8.45
−11.27


Moons: Decision function (linear kernel)
Data points
Training
Test
4.344
3.258
2.172
1.086
0.000
−1.049
−2.098
−3.147
−4.196