KernelCourse2020_Exercise03

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1 Exercise 03

Kernel Methods in Machine Learning (CS-E4830)

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Tasks:

1. Section **??**
2. Section **??** (**2 Points**)
3. Section **??** (**3 Point**)
4. Section **??**
5. Section **??**
6. Section **??** (**1 Point**)
7. Section **??** (**1 Point**)

8. Section **??** (**1 point**)

Version: 1.3

Version history:

- 1.0: Initial version
- 1.1: Modify SVM class: For $|\alpha_i - C| < \epsilon$ we set $\alpha_i = C$. This fix improves the numerical stability of the SVM Section **??**.
- 1.2: Minor changes: Fix doc-string of `decision_function`, rename `self._ytrain` to `self._y_train` in `__init__`, and indicate what is the Section **??**
- 1.3: Modify the points for comparison to LinSVM

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

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[1]:
```
import time

import numpy as np
import scipy.optimize as spopt
```

```
import matplotlib.pyplot as plt

from sklearn.base import BaseEstimator, ClassifierMixin
from sklearn.model_selection import train_test_split, GridSearchCV, KFold
from sklearn.svm import SVC as SVM_sk
from sklearn.datasets import make_blobs, make_moons
from sklearn.metrics.pairwise import rbf_kernel as rbf_kernel_sk
from sklearn.metrics.pairwise import linear_kernel as linear_kernel_sk
```

[2]:
```
def gaussian_kernel_wrapper(X, Y=None, sigma=None):
    """
    Wrapper around the sklearn rbf-kernel function. It converts between the
    gamma parametrization (sklearn) and the sigma parametrization (lecture).
    """
    if sigma is None:
        sigma = np.sqrt(X.shape[1] / 2.)

    return rbf_kernel_sk(X, Y, gamma=(1. / (2. * (sigma**2))))
```

[3]:
```
def plot_svm_model(X, y, svm, ax=None, show_origin=False, verbose=True):
    """
    Helper function to plot svm models for simple 2D-data.
    """
    # Fit model
    svm.fit(X, y)

    if verbose:
        if isinstance(svm, SVM_sk):
            print("Number of support vectors:", svm.n_support_)
            print("Bias:", np.round(svm.intercept_, 4))
        else:
            print("Number of support vectors:", svm.n_sv)
            print("Bias:", np.round(svm._bias, 4))
            print("Dual variables:\n", np.round(svm._alpha[svm._alpha > 0], 4))

    if ax is None:
        fig = plt.figure()
        ax = fig.add_subplot(111)

    _ = ax.scatter(X[y == 1, 0], X[y == 1, 1], c="blue", s=50, label="positive␣
↪class")
    _ = ax.scatter(X[y == -1, 0], X[y == -1, 1], c="red", s=50, label="negative␣
↪class")

    # plot the decision function
    xlim = ax.get_xlim()
    ylim = ax.get_ylim()
```

```
    if show_origin:
        xlim = (np.minimum(-0.5, xlim[0]), np.maximum(0.5, xlim[1]))
        ylim = (np.minimum(-0.5, ylim[0]), np.maximum(0.5, ylim[1]))

        ax.plot(0, 0, 's', c="k", label="Origin")

    # create grid to evaluate model
    xx = np.linspace(xlim[0], xlim[1], 30)
    yy = np.linspace(ylim[0], ylim[1], 30)
    YY, XX = np.meshgrid(yy, xx)
    xy = np.vstack([XX.ravel(), YY.ravel()]).T
    Z = svm.decision_function(xy).reshape(XX.shape)

    # plot decision boundary and margins
    _ = ax.contour(XX, YY, Z, colors='k', levels=[-1, 0, 1], alpha=0.5,
                   linestyles=['--', '-', '--'])
    # plot support vectors
    _ = ax.scatter(svm.support_vectors_[:, 0], svm.support_vectors_[:, 1],␣
↪s=200,
                   linewidth=1.5, facecolors='none', edgecolors='k',␣
↪label="Support vectors")
    _ = ax.legend()

    _ = ax.grid()
```

1.1 1. C - Support Vector Machine (C-SVM)

In this task you are going to implement a soft-margin C-SVM. You will use the dual formulation (derived in the Pen & Paper exercise) to find the optimal model using quadratic programming (QP).

SciPy Optimization Toolbox A convenient interface to a QP-solver is provided by the scipy.optimization package (JupyterHub uses version 1.1.0). As optimization algorithm we will use Sequential Least SQuares Programming (SLSQP) (`scipy.optimize.minimize(..., method="SLSQP")`). Another popular framework for optimization in Python is, e.g., cvxpy (not available on JupyterHub).

SVM Primal formulation For a given training set $\{(\mathbf{x}_i, y_i)\}_{i=1}^{n_{train}}$, the C-SVM formulation is given as:

$$\min_{\mathbf{w},\boldsymbol{\xi},b} \frac{1}{2}\|\mathbf{w}\|^2 + C \sum_{i=1}^{n_{train}} \xi_i \tag{1}$$

$$\text{s.t. } y_i(\mathbf{w}^T\phi(\mathbf{x}_i)) + b) \geq 1 - \xi_i \tag{2}$$

$$\xi_i \geq 0, \quad i = 1, \ldots, n_{train}, \tag{3}$$

where $\mathbf{w} \in \mathbb{R}^d$ are the model parameters, and $b \in \mathbb{R}$ is the bias, and $\boldsymbol{\xi} \in \mathbb{R}^{n_{train}}_{\geq 0}$ is the vector of slack-variables, and $C > 0 \in \mathbb{R}$ is the regularization parameter.

The primal C-SVM **decision function** is given as:

$$f(\mathbf{x}) = \mathbf{w}^T\phi(\mathbf{x}) + b \in \mathbb{R}$$

and the corresponding **prediction function** as:

$$g(\mathbf{x}) = sign(f(\mathbf{x})) \in \{-1, 1\}.$$

SVM Dual formulation In the Pen & Paper exercise you showed, that the dual C-SVM can be written as:

$$\max_{\boldsymbol{\alpha}} \mathcal{L}(\boldsymbol{\alpha}) = \underbrace{\sum_{i=1}^{n_{train}} \alpha_i - \frac{1}{2} \sum_{i=1}^{n_{train}} \sum_{j=1}^{n_{train}} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j)}_{\text{Loss function}} \tag{4}$$

$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, n_{train} \tag{5}$$

$$\underbrace{\sum_{i=1}^{n_{train}} \alpha_i y_i = 0,}_{\text{Bias constraint}} \tag{6}$$

or, equivalent in matrix notation, as:

$$\max_{\boldsymbol{\alpha}} \mathbf{1}^T\boldsymbol{\alpha} - \frac{1}{2}\boldsymbol{\alpha}^T \left(\mathbf{y}\mathbf{y}^T \circ \mathbf{K}\right) \boldsymbol{\alpha} \tag{7}$$

$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad i = 1, \ldots, n_{train} \tag{8}$$

$$\boldsymbol{\alpha}^T\mathbf{y} = 0, \tag{9}$$

where $\boldsymbol{\alpha} \in \mathbb{R}^{n_{train}}$ are the dual variables, and $\mathbf{K} \in \mathbb{R}^{n_{train} \times n_{train}}$ is the training kernel matrix (with $[\mathbf{K}]_{ij} = \kappa(\mathbf{x}_i, \mathbf{x}_j) = \phi(\mathbf{x}_i)^T\phi(\mathbf{x}_j)$), and $\mathbf{y} \in \{-1, 1\}^{n_{train}}$ training labels, and $C > 0 \in \mathbb{R}$ being the regularisation parameter. Let us furthermore define the shorthand: $\mathbf{G} = \mathbf{y}\mathbf{y}^T \circ \mathbf{K}$.

Support Vector (SV) The training examples $\mathbf{x}_i$ (respectively their feature vectors $\phi(\mathbf{x}_i)$) for which $\alpha_i > 0$ are called **support vectors (SV)**. The examples $\mathbf{x}_i$ for which *additionally* holds $\alpha_i < C$ are the SVs **on the margin**. For convenience let us define $\mathcal{I}_S$ being the index set of the support vectors and $\mathcal{I}_M$ being the index set of the support vectors on the margin. ##### Dual C-SVM **decision function**

The Dual C-SVM decision function for a new exmaple $\mathbf{x}$ can be written as:

$$f(\mathbf{x}) = \left(\sum_{i=1}^{n_{train}} \alpha_i y_i \kappa(\mathbf{x}, \mathbf{x}_i) \right) + b = \left(\sum_{i \in \mathcal{I}_S} \alpha_i y_i \kappa(\mathbf{x}, \mathbf{x}_i) \right) + b \in \mathbb{R}$$

or, equivalent in matrix notation, as:

$$f(\mathbf{x}) = \left(\mathbf{y}[\mathcal{I}_S] \circ \boldsymbol{\alpha}[\mathcal{I}_S] \right)^T \mathbf{k}(\mathbf{x})[\mathcal{I}_S] + b,$$

with $z[\cdot]$ element access similar to numpy, and $\mathbf{k}(\mathbf{x}) = [\kappa(\mathbf{x}, \mathbf{x}_1), \ldots, \kappa(\mathbf{x}, \mathbf{x}_{n_{train}})] \in \mathbb{R}^{n_{train}}$ are the kernel values between the new and the training examples.

Estimating the Bias-term b For the SVs on the margin we know that $\xi_i = 0$ and therefore that $y_i f(\mathbf{x}_i) = 1$. We can therefore calculate b for a given $\boldsymbol{\alpha}$ using:

$$b = \frac{1}{|\mathcal{I}_M|} \sum_{i \in \mathcal{I}_M} \left(y_i - \sum_{j \in \mathcal{I}_s} y_j \alpha_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \right)$$

or, equivalent in matrix notation:

$$b = \frac{1}{|\mathcal{I}_M|} \mathbf{1}^T \left(\mathbf{y}[\mathcal{I}_M] - \mathbf{K}[\mathcal{I}_M][:, \mathcal{I}_S] \left(\mathbf{y}[\mathcal{I}_S] \circ \boldsymbol{\alpha}[\mathcal{I}_S] \right) \right).$$

For further details, check out "Pattern Recognition and Machine Learning" book by C. Bishop (p. 333-334).

1.1.1 A. Dual optimization using quadratic programming (QP) (2 Points)

```
<b>Task:</b>
Implement missing code parts of the SVM class. You have to modify the following member-functio
```

- `_loss_and_grad`: This function should return the loss function value $\mathcal{L}(\boldsymbol{\alpha})$ for a given $\boldsymbol{\alpha}$ vector and the gradient $\nabla_{\boldsymbol{\alpha}} \mathcal{L}$ of the loss function.
- `_calculate_bias`: This function should return the bias calculated as Section **??**. Keep the Section **??** in mind.
- `fit`: In this function you need to define the $\mathbf{G}$ matrix, the box and linear constraints (*s.t.*) and run the optimizer.
- `decision_function` and `predict`: This functions should implement the functions $f(\mathbf{x})$ and $g(\mathbf{x})$.

Hints / Notes:

- There are online tools existing to check your derived gradients, e.g. matrixcalculus.org.
- Make your self familiar with the `scipy.optimize.minimize` function.
- Read how to define box- (bounds) and linear-constraints?
- The dual loss function $\mathcal{L}$ can be maximized by minimizing $-\mathcal{L}$. Scipy only implements a minimize function.
- Section **??** might help you debugging it.
- Instead of the index sets $\mathcal{I}_M$ and $\mathcal{I}_S$, the implementation works with indicator vectors, e.g. `_is_sv$ ={True,False}^{n_{train}}$` with `_is_sv[i]` $= \alpha_i > 0$.

[166]:
```
class SVM(BaseEstimator, ClassifierMixin):
    def __init__(self, C=1., alpha_threshold=1e-6, sigma=None,␣
↪kernel="gaussian", verbose=True):
        """
        C - Support Vector Machine (SVM)

        :param C: scalar, regularization parameter C (default = 1)
        :param alpha_threshold: scalar, threshold to set the dual variables to␣
↪zero if very
            small (e.g. due to numerical optimization) (default = 1e-6)
        :param sigma: scalar, sigma parameter used for the gaussian kernel␣
↪(default = None)
        :param kernel: {string, calaable}, name of the kernel to use or␣
↪function to
            calculate the kernel matrices (defualt = "gaussian")
        :param verbose: boolean, indicating whether some performance /␣
↪debugging information
            should be plotted
        """
        # Optimization parameters
        self.C = C
        self._alpha_threshold = alpha_threshold
        self._verbose = verbose

        # Model parameters
        self._alpha = None      # dual variables alpha_i
        self._bias = None       # bias term
        self._X_train = None    # training feature vectors needed for prediction
        self._y_train = None     # training labels

        # Support vector information
        self._is_sv = None            # indicator vector, which example is␣
↪support vector
        self.n_sv = None              # number of support vectors per class
        self.support_vectors_ = None  # Support vector input feature vectors
```

```
        # Kernel parameters
        self.kernel = kernel
        self.sigma = sigma

    def _loss_and_grad(self, alpha, G, sign=-1):
        """
        Calculate the SVM dual loss function and its corresponding gradient.

        :param alpha: array-like, shape=(n_train, ), current dual variable␣
↪vector
        :param G: array-like, shape=(n_train, n_train), G_train matrix
        :param sign: scalar, sign of the loss and gradient, should be 1 for␣
↪minimization and
            -1 for maximization (default = -1)

        :return tuple=(loss function value, gradient vector [shape=(n_train,)])
        """
        # YOUR CODE HERE
        loss_value = np.sum(alpha) - 0.5*np.dot( np.dot(alpha.reshape(-1,1).T,␣
↪G), alpha.reshape(-1,1) )[0,0]
        gradient_vector = 1 - np.dot(G,alpha).flatten()
        #print("loss: ", loss_value)
        #print("gradient: ", gradient_vector)
        #raise NotImplementedError()

        return sign * loss_value, sign * gradient_vector

    def _calculate_bias(self, K_train, y_train, alpha, is_sv):
        """
        Function to determine the bias term after the dual variables have been␣
↪optimized.

        :param K_train: array-like, shape=(n_train, n_train), training kernel␣
↪matrix
        :param y_train: array-like, shape=(n_train, 1), training labels
        :param alpha: array-like, shape=(n_train,), dual variables
        :param is_sv: array-like, shape=(n_train,), boolean vector indicating␣
↪whether a
            training example is a support vector or not, i.e. is_cv[i] == True␣
↪=> alpha[i] > 0

        :return: scalar, bias
        """
        # Get indicator vector of the support vectors on the margin,
        # i.e. for which slack_i = 0.
        is_sv_mrg = np.bitwise_and(is_sv, (alpha < self.C).flatten())
```

```
        # Calculate the bias according to the formula.
        # YOUR CODE HERE

        size_mrg = np.sum(is_sv_mrg)
        bias = np.sum(y_train[is_sv_mrg]- K_train[is_sv_mrg][:, is_sv]@(np.
↪multiply(y_train[is_sv], alpha[is_sv]) ))/size_mrg

        #raise NotImplementedError()

        return bias

    def fit(self, X_train, y_train):
        """
        Fit the SVM model parameters

        :param X_train: array-like, shape=(n_train, n_features), training␣
↪feature matrix
        :param y_train: array-like, shape=(ntrain, ) or (n_train, 1), training␣
↪labels, {-1, 1}

        :return: reference to it self
        """
        self._X_train = X_train
        K_train = self._get_kernel(self._X_train)
        n_train = K_train.shape[0]  # number of training examples

        # Make training labels beeing a column-vector
        self._y_train = y_train
        if len(self._y_train.shape) == 1:
            self._y_train = self._y_train[:, np.newaxis]

        # Calculate the matrix: G_train = yy' .* K_train
        # YOUR CODE HERE
        G_train = np.multiply(self._y_train@(self._y_train.T), K_train)
        #raise NotImplementedError()

        # Set up the equality contraint introduced by the bias-term: bias_const
        # YOUR CODE HERE
        bias_const = {}
        bias_const['type'] = 'eq'
        bias_const['fun'] = lambda x: (self._y_train.T)@x
        #raise NotImplementedError()

        assert (isinstance(bias_const, dict) and \
                "type" in bias_const and \
                "fun" in bias_const), \
```

```
            "bias_const must be specified as dictionary. See hints."
        assert (callable(bias_const["fun"])), "Provide a function to evalute␣
↪the constraint."

        # Define the bounds (0 <= alpha_i <= C) for the dual varaibles:␣
↪bound_const
        # YOUR CODE HERE
        bounds_const = spopt.Bounds(np.zeros(n_train,), self.C *np.
↪ones(n_train,))
        #raise NotImplementedError()

        assert (isinstance(bounds_const, spopt.Bounds))

        # Define a feasiable initial value for the dual variables:
        # 0 <= alpha0_i <= C, y^T alpha0_i = 0
        # YOUR CODE HERE
        alpha0 = np.zeros(n_train,)
        #raise NotImplementedError()

        assert (alpha0.shape == (n_train, )), "alpha0 must have␣
↪shape=(n_train,)."
        assert (all(alpha0 >= 0) and all(alpha0 <= self.C) and (self._y_train.T␣
↪@ alpha0 == 0)), \
            "alpha0 must be feasible."

        if self._verbose:
            start = time.time()

        # Run the optimizer
        res = spopt.minimize(self._loss_and_grad, x0=alpha0, jac=True,␣
↪args=(G_train, ),
                             method="SLSQP", constraints=bias_const,␣
↪bounds=bounds_const)

        if self._verbose:
            print("Optimizing time: %.3fs" % (time.time() - start))

        # Extract the optimal dual varaibles (solution) from the optimizer
        self._alpha = res["x"][:, np.newaxis]

        # Threshold alpha values to zero if very small
        self._alpha[self._alpha < self._alpha_threshold] = 0
        self._alpha[np.abs(self._alpha - self.C) < self._alpha_threshold] =␣
↪self.C

        # Find support vectors (alpha_i > 0)
```

```
        # YOUR CODE HERE
        self._is_sv = self._alpha.flatten()>0
        #raise NotImplementedError()

        assert (self._is_sv.shape == (n_train, )), \
            "_is_sv must be an indicator vector with shape=(n_train, )."

        self.support_vectors_ = X_train[self._is_sv]

        # Get number of support vectors per class
        self.n_sv = np.array([np.sum(self._is_sv[y_train.flatten() == -1]),
                              np.sum(self._is_sv[y_train.flatten() ==  1])])

        # Calcualte the bias
        self._bias = self._calculate_bias(K_train, self._y_train, self._alpha,␣
↪self._is_sv)

        return self

    def decision_function(self, X):
        """
        Calculate decision function:
            f(x) = sum_i y_i alpha_i k(x_i, x) + bias

        :param X: array-like, shape=(n_test, n_features),
        :return: array-like, shape=(n_test, ), decision function value f(x) for␣
↪all test
            samples
        """
        # Calculate the test-training kernel shape=(n_test, n_train)
        K_test_train = self._get_kernel(X, self._X_train)
        #print("K_test_train.shape: ", K_test_train.shape)

        # Calculate the decision function values (only using SV)
        # YOUR CODE HERE
        g_X = (K_test_train@(np.multiply(self._y_train,self._alpha))) + self.
↪_bias
        #raise NotImplementedError()

        # reduce to 1d vector
        g_X = g_X.flatten()

        # check output dimension
        assert (g_X.shape == (X.shape[0], )), \
            "Output of the decision function must have shape: (n_test, )"

        return g_X
```

```
    def predict(self, X):
        """
        Predict labels using C-SVM:
            g(x) = sign(f(x)), with f(x) being the decision function

        :param X: array-like, shape=(n_test, n_features), test feature matrix
        :return: array-like, shape=(n_test,), predicted labels {-1, 1} for all␣
↪test samples
        """
        # YOUR CODE HERE
        y_X = np.sign(self.decision_function(X))
        #raise NotImplementedError()

        assert ((np.in1d(y_X, [-1, 0, 1]).all())), \
            "Output of the prediction function must be {-1, 0, 1}"

        return y_X

    def _get_kernel(self, X, Y=None):
        """
        Caculate 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_wrapper(X, Y, self.sigma)
        elif self.kernel == "linear":
            return linear_kernel_sk(X, Y)
        elif callable(self.kernel):
            return self.kernel(X, Y)
        else:
            raise ValueError("Invalid kernel chosen.")
```

Tests for the _loss_and_grad Function

[167]:
```
# Tests for the loss & gradient function

# Very simple data
# __X = np.array([[0, 1], [-1, 0], [0, -1], [1, 0]])
# __y = np.array([1, 1, -1, -1])
```

```
# Linear kernel
__G = np.array([[1, 0, 1, 0], [0, 1, 0, 1], [1, 0, 1, 0], [0, 1, 0, 1]])  # assume linear K
__alpha = np.full((4, ), 0.5)
__loss_val, __grad_vec = SVM(C=1.)._loss_and_grad(__alpha, __G)

assert (np.isscalar(__loss_val)), "Loss value must be a scalar."
assert (__grad_vec.shape == __alpha.shape), "Gradient vector must have same length as alpha."

np.testing.assert_allclose(__loss_val, - (2. - 0.5 * 2.),
                           err_msg="Loss value is wrong.")  # remember the negative sign of loss
np.testing.assert_allclose(__grad_vec, np.zeros((4, )),
                           err_msg="Gradient vector is wrong.")

# Gaussian kernel
__G = np.array([[ 1.   ,  0.368,  0.135,  0.368],
                [ 0.368,  1.   ,  0.368,  0.135],
                [ 0.135,  0.368,  1.   ,  0.368],
                [ 0.368,  0.135,  0.368,  1.   ]])  # assume gaussian K
__alpha = np.ones((4, ))
__loss_val, __grad_vec = SVM(C=1., kernel="gaussian")._loss_and_grad(__alpha, __G)

np.testing.assert_allclose(__loss_val, - (4. - 0.5 * 7.484),
                           err_msg="Loss value is wrong.")  # remember the negative sign of loss
np.testing.assert_allclose(__grad_vec, np.full((4, ), 0.871),
                           err_msg="Gradient vector is wrong.")
```

Tests for the _calculate_bias Function

[168]:
```
# Test for the bias calculation

# Simple data (linear separable)
__X = np.array([[-1, 0], [0, 1], [-.75, .75], [0, -1], [1, 0]])
__y = np.array([1, 1, 1, -1, -1])
__C = 10.

# Get dual variable vector using the sklearn SVM
__svm_sk = SVM_sk(C=__C, kernel="linear").fit(__X, __y)
__alpha = np.zeros((__X.shape[0], ))
# Note: Sklearn stores only dual_coef_i = alpha_i * y_i
__alpha[__svm_sk.support_] = __svm_sk.dual_coef_ * __y[__svm_sk.support_]
```

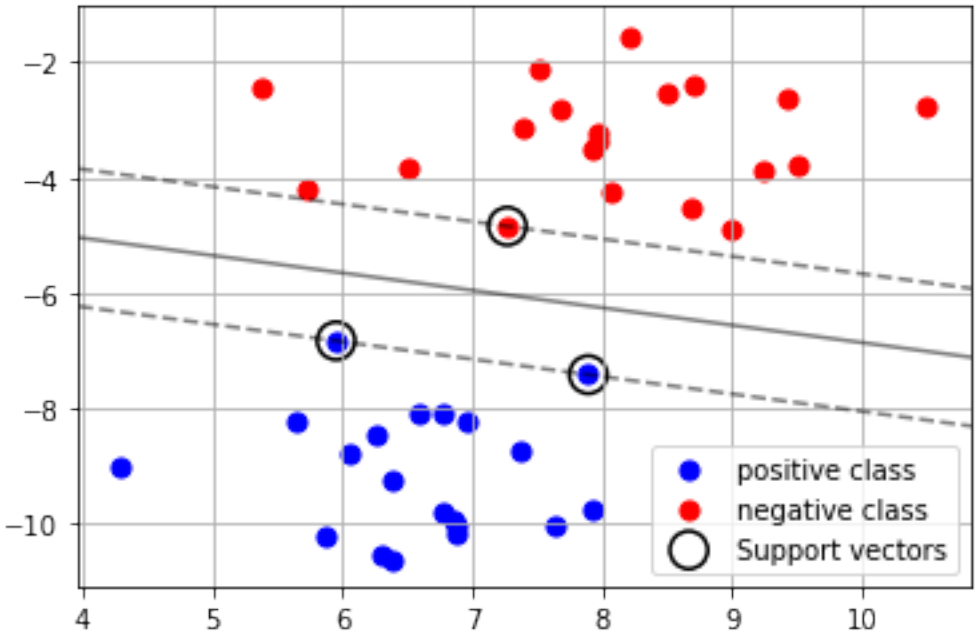
```
# Determine support vectors
__is_sv = (__alpha > 0)

# Calculate the bias
__bias = SVM(C=__C, kernel="linear")._calculate_bias(linear_kernel_sk(__X), __y,
                                                     __alpha, __is_sv)
np.testing.assert_array_equal(__bias, __svm_sk.intercept_, err_msg="Bias term␣
 ↪is not correct.")

# Simple data (linear separable): shifted data
# Get dual variable vector using the sklearn SVM
__X += np.array([-1., 1.])
__svm_sk = SVM_sk(C=__C, kernel="linear").fit(__X, __y)
__alpha = np.zeros((__X.shape[0], ))
__alpha[__svm_sk.support_] = __svm_sk.dual_coef_ * __y[__svm_sk.support_]

# Determine support vectors
__is_sv = (__alpha > 0)

# Calculate the bias
__bias = SVM(C=__C, kernel="linear")._calculate_bias(linear_kernel_sk(__X),
                                                     __y, __alpha, __is_sv)
np.testing.assert_array_equal(__bias, __svm_sk.intercept_, err_msg="Bias term␣
 ↪is not correct.")

# Simple data (not separable)
__X = np.array([[-1, 0], [0, 1], [.75, -.75], [0, -1], [1, 0]]) + np.array([-1.
 ↪, 1.])
__y = np.array([1, 1, 1, -1, -1])
__C = 10.

# Get dual variable vector using the sklearn SVM
__svm_sk = SVM_sk(C=__C, kernel="linear").fit(__X, __y)
__alpha = np.zeros((__X.shape[0], ))
__alpha[__svm_sk.support_] = __svm_sk.dual_coef_ * __y[__svm_sk.support_]

# Determine support vectors
__is_sv = (__alpha > 0)

# Calculate the bias
__bias = SVM(C=__C, kernel="linear")._calculate_bias(linear_kernel_sk(__X), __y,
                                                     __alpha, __is_sv)
np.testing.assert_allclose(__bias, __svm_sk.intercept_,
                           err_msg="Bias term is not correct.", atol=1e-6)
```

Visual Inspection of your C-SVM Implementation Here we run a small classification problem, that is linearly seperable. The example is taken from the sklearn-package Maximum margin separating hyperplane example. Your model should have *three* support vectors (one red -, two blue +). Your estimated bias should $b = -3.2145$ and your dual variables (of the support vectors, i.e. $\alpha_i > 0$) $\boldsymbol{\alpha} = [0.3834, 0.2537, 0.1297]^T$.

Note: Here for first time we actually run to optimizer. So if anything goes wrong, chec

[170]:
```
# Create some very simple test data
X, y = make_blobs(n_samples=40, centers=2, random_state=6)
y[y==0] = -1
plot_svm_model(X, y, SVM(C=1, kernel="linear", verbose=False))
```

```
Number of support vectors: [1 2]
Bias: -3.2145
Dual variables:
 [0.3834 0.2537 0.1297]
```



1.1.2 B. Comparison to Sklearn SVM (libSVM) (1 Point)

In this task your SVM implementation will be applied on two artificial datasets (see also exericse 1) and compared with the performance of the sklearn SVC implementation. Sklearn uses libSVM as solver in the background. If you are interested in SVM solver implementation details, you can read the libSVM manual.

Task: Your SVM implentation is applied here, i.e. do not need to write additional

[171]:
```
# Test implementation agains sklearn
__X_blobs, __y_blobs = make_blobs(n_samples=350, centers=[[1, 1], [3, 3]],
                                  cluster_std=[0.5, 1.15], random_state=202)
__X_moons, __y_moons = make_moons(n_samples=350, noise=0.25, random_state=212)

# 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=191)
__X_moons_train, __X_moons_test, __y_moons_train, __y_moons_test =␣
 ↪train_test_split(
    __X_moons, __y_moons, random_state=881)

# Blobs
print("Blobs:", end="\n\t")
__svm_sk = SVM_sk(C=2., kernel="rbf", gamma="auto").fit(__X_blobs_train,␣
 ↪__y_blobs_train)
__svm = SVM(C=2., kernel="gaussian").fit(__X_blobs_train, __y_blobs_train)

print("\tTest score (sklearn, scipy):",
      np.round(__svm_sk.score(__X_blobs_test, __y_blobs_test), 3),
      np.round(__svm.score(__X_blobs_test, __y_blobs_test), 3))
print("\tN_sv (sklearn, scipy):", __svm_sk.n_support_, __svm.n_sv)
print("\tBias (sklearn, scipy):", np.round(__svm_sk.intercept_, 3), np.
 ↪round(__svm._bias, 3))

np.testing.assert_allclose(__svm.score(__X_blobs_test, __y_blobs_test),
                           __svm_sk.score(__X_blobs_test, __y_blobs_test),
                           err_msg="Blobs: Test set accuracies differ too much.
 ↪")
np.testing.assert_equal(__svm.n_sv, __svm_sk.n_support_,
                        err_msg="Moons: Number of support vectors does not␣
 ↪match.")
np.testing.assert_allclose(__svm._bias, __svm_sk.intercept_, atol=1e-2,
                           err_msg="Blobs: Bias values differ too much.")

# Moons
print("Moons:", end="\n\t")
__svm_sk = SVM_sk(C=2., kernel="rbf", gamma="auto").fit(__X_moons_train,␣
 ↪__y_moons_train)
__svm = SVM(C=2., kernel="gaussian").fit(__X_moons_train, __y_moons_train)
```

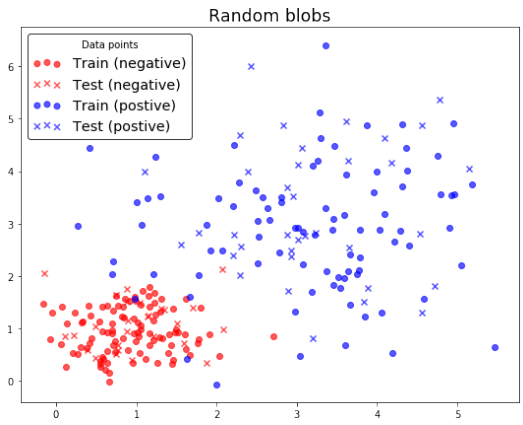
```
print("\tTest score (sklearn, scipy):",
      np.round(__svm_sk.score(__X_moons_test, __y_moons_test), 3),
      np.round(__svm.score(__X_moons_test, __y_moons_test), 3))
print("\tN_sv (sklearn, scipy):", __svm_sk.n_support_, __svm.n_sv)
print("\tBias (sklearn, scipy):", np.round(__svm_sk.intercept_, 3), np.
 ↪round(__svm._bias, 3))

np.testing.assert_allclose(__svm.score(__X_moons_test, __y_moons_test),
                           __svm_sk.score(__X_moons_test, __y_moons_test),
                           err_msg="Moons: Test set accuracies differ too much.
 ↪")
np.testing.assert_equal(__svm.n_sv, __svm_sk.n_support_,
                        err_msg="Moons: Number of support vectors does not␣
 ↪match.")
np.testing.assert_allclose(__svm._bias, __svm_sk.intercept_, atol=1e-2,
                           err_msg="Moons: Bias values differ too much.")
```

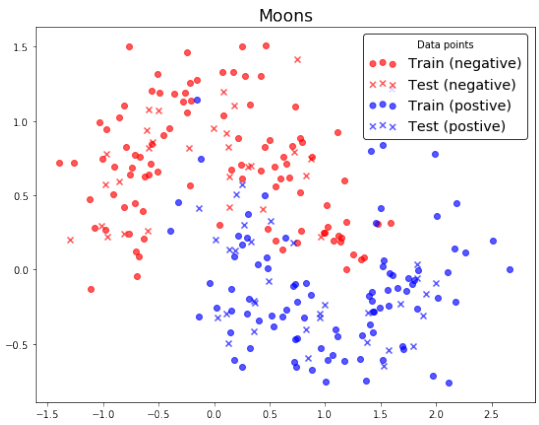
```
Blobs:
        Optimizing time: 4.405s
        Test score (sklearn, scipy): 0.966 0.966
        N_sv (sklearn, scipy): [14 23] [14 23]
        Bias (sklearn, scipy): [0.624] 0.624
Moons:
        Optimizing time: 4.318s
        Test score (sklearn, scipy): 0.932 0.932
        N_sv (sklearn, scipy): [41 40] [41 40]
        Bias (sklearn, scipy): [0.081] 0.082
```

1.1.3 C. Visualization of the Model and Support Vectors

[172]:
```
# Create synthetic data (Please do not change the random_state!)
X_blobs, y_blobs = make_blobs(n_samples=250, centers=[[1, 1], [3, 3]],␣
 ↪cluster_std=[0.5, 1.15], random_state=202)
X_moons, y_moons = make_moons(n_samples=250, noise=0.25, random_state=211)
# 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=191)
X_moons_train, X_moons_test, y_moons_train, y_moons_test =␣
 ↪train_test_split(X_moons, y_moons, random_state=881)
```

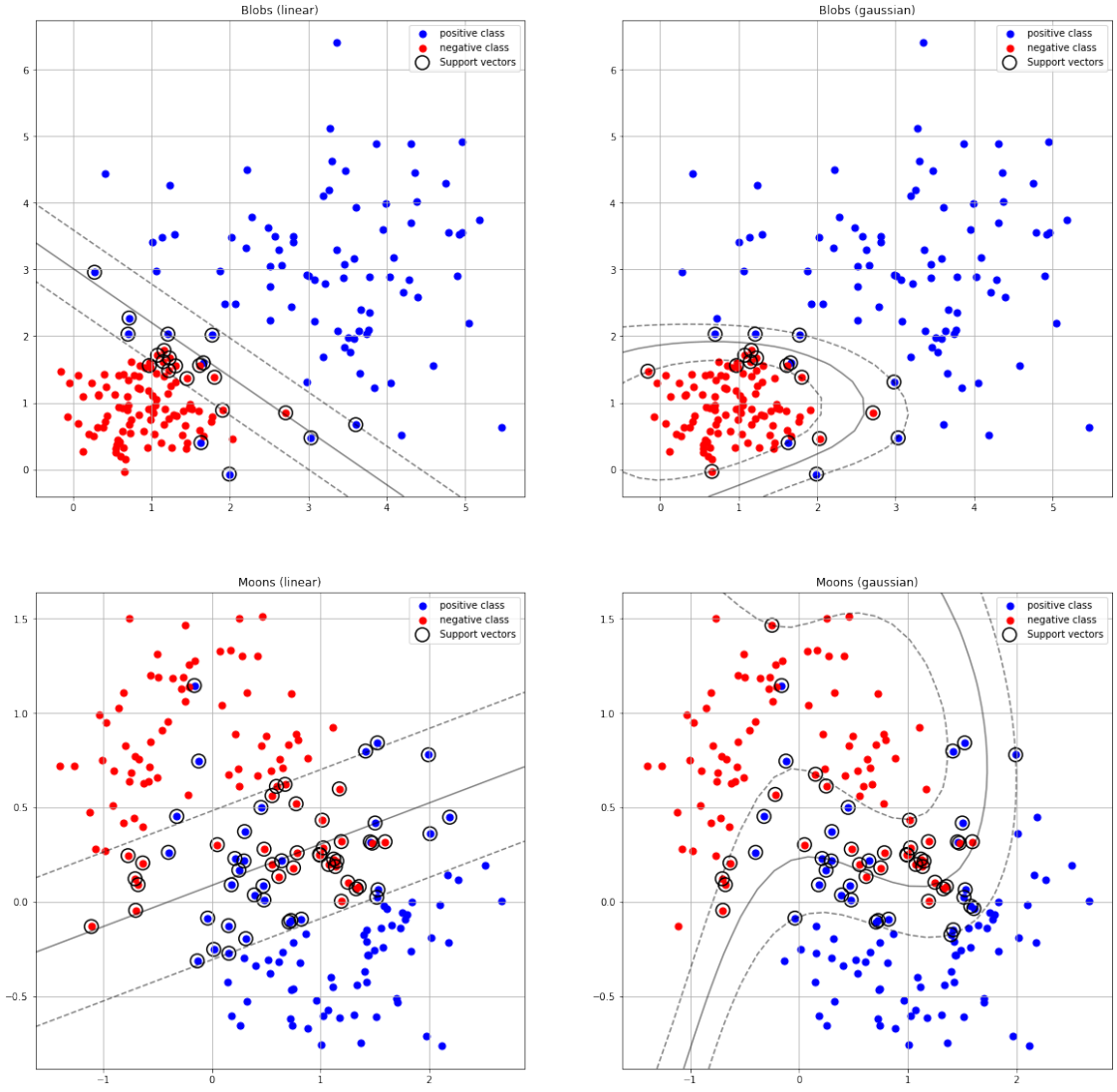
[173]:
```
# Plot datasets
fig, axrr = plt.subplots(1, 2, figsize=(20, 7))

# Blobs
for l_str, l_num, col in [("negative", -1, "red"), ("postive", 1, "blue")]:
    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)

    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, "red"), ("postive", 1, "blue")]:
    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)

    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()
```





[174]:
```
fig, axrr = plt.subplots(2, 2, figsize=(20, 20))
plot_svm_model(X_blobs_train, y_blobs_train, SVM(C=10., kernel="linear"),
               ax=axrr[0, 0], verbose=False)
axrr[0, 0].set_title("Blobs (linear)")
plot_svm_model(X_blobs_train, y_blobs_train, SVM(C=10., kernel="gaussian",␣
 ↪sigma=1.5),
               ax=axrr[0, 1], verbose=False)
axrr[0, 1].set_title("Blobs (gaussian)")
plot_svm_model(X_moons_train, y_moons_train, SVM(C=10., kernel="linear"),
               ax=axrr[1, 0], verbose=False)
axrr[1, 0].set_title("Moons (linear)")
plot_svm_model(X_moons_train, y_moons_train, SVM(C=10., kernel="gaussian",␣
 ↪sigma=1.5),
               ax=axrr[1, 1], verbose=False)
_ = axrr[1, 1].set_title("Moons (gaussian)")
```

```
Optimizing time: 1.386s
Optimizing time: 1.576s
Optimizing time: 1.344s
Optimizing time: 1.485s
```



1.2 2. Non-linear Kernels

In this task you are going to implement two non-linear hyper-parameter free kernels for binary and non-negative feature vectors. Assume, we are given 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.

1.2.1 A. Tanimoto-Kernel for Binary Data (1 Point)

The tanimoto kernel is used to calculate the similarities for binary input data. It calculates the normalized intersection between two sets and is also known as Jaccard Index.

Task:

Implement missing code parts of the function calculation the Tanimoto kernel matrix given two i

$$[\mathbf{K}_{tan}]_{ij} = \kappa_{tan}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\mathbf{x}_i^T \mathbf{x}_j}{\mathbf{x}_i^T \mathbf{x}_i + \mathbf{x}_j^T \mathbf{x}_j - \mathbf{x}_i^T \mathbf{x}_j},$$

where $\mathbf{x}_i, \mathbf{x}_j \in \{0,1\}^d$ are two binary vectors from set A respectively B.

Note that, the kernel values are normalized, i.e. $\kappa_{tan}(\mathbf{x}_i, \mathbf{x}_j) \in [0,1]$.

[205]:
```
def tanimoto_kernel(X, Y=None):
    """
    Tanimoto kernel function

    :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), tanimoto kernel matrix
    """
    if Y is None:
        Y = X

    # YOUR CODE HERE
    diag_A = np.diag(X@X.T).reshape(-1,1)
    diag_B=  np.diag(Y@Y.T).reshape(1,-1)
    sum_A_B = diag_A+diag_B
    K = X@Y.T / (sum_A_B-X@Y.T)
    #raise NotImplementedError()
    return K
```

[207]:
```
__X_A = np.array([[1, 1, 0], [0, 1, 1], [1, 0, 0]])
__X_B = np.array([[1, 0, 1], [1, 1, 1], [0, 0, 0], [1, 1, 0]])

# symmetric kernel
__K = tanimoto_kernel(__X_A)
np.testing.assert_equal(__K.shape, (3, 3))
np.testing.assert_equal(np.diag(__K), np.ones((3, )))
np.testing.assert_equal(__K[0, 1], 1. / 3.)
np.testing.assert_equal(__K[1, 0], 1. / 3.)
np.testing.assert_equal(__K[0, 2], 1. / 2.)
np.testing.assert_equal(__K[2, 0], 1. / 2.)
assert(np.max(__K) <= 1.), "Kernel values must be <= 1"
assert(np.min(__K) >= 0.), "Kernel values must be >= 0"

# non-symmetric kernel
```

```
__K = tanimoto_kernel(__X_A, __X_B)
np.testing.assert_equal(__K.shape, (3, 4))
np.testing.assert_equal(__K[0, 1], 2. / 3.)
np.testing.assert_equal(__K[1, 0], 1. / 3.)
np.testing.assert_equal(__K[0, 2], 0.)
np.testing.assert_equal(__K[2, 0], 1. / 2.)
assert(np.max(__K) <= 1.), "Kernel values must be <= 1"
assert(np.min(__K) >= 0.), "Kernel values must be >= 0"
```

1.2.2 B. MinMax-Kernel for Non-negative Data (1 Point)

The MinMax-Kernel is a normalized formulation of the intersection kernel for non-negative data, e.g. popular in image-processing and for counting data.

Task:

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

$$[\mathbf{K}_{minmax}]_{ij} = \kappa_{minmax}(\mathbf{x}_i, \mathbf{x}_j) = \frac{\sum_{s=1}^{d} \min(\mathbf{x}_i^{(s)}, \mathbf{x}_j^{(s)})}{\sum_{s=1}^{d} \max(\mathbf{x}_i^{(s)}, \mathbf{x}_j^{(s)})},$$

where $\mathbf{x}_i, \mathbf{x}_j \in \mathbb{N}_0^d$ are two non-negative feature vectors.

Note, the kernel values are normalized, i.e. $\kappa_{minmax}(\mathbf{x}_i, \mathbf{x}_j) \in [0, 1]$.

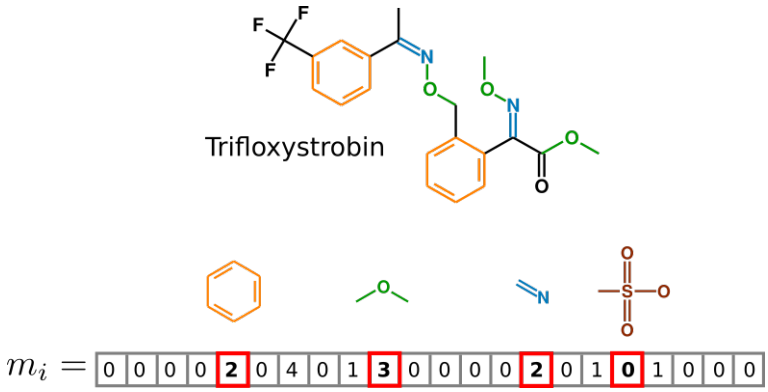
[220]:
```
def minmax_kernel(X, Y=None):
    """
    Min-Max kernel function

    :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), minmax kernel matrix
    """
    if Y is None:
        Y = X

    n_A, n_B = X.shape[0], Y.shape[0]

    # YOUR CODE HERE
    K = np.zeros((n_A,n_B))
    for i in range(n_A):
```

```
        for j in range(n_B):
            denom = np.sum( np.maximum(X[i],Y[j]) )
            num = np.sum( np.minimum(X[i],Y[j]) )
            K[i,j] = num/denom
    #raise NotImplementedError()

    return K
```

[221]:
```
# Test on some small data
__X_A = np.array([[0, 1, 2], [1, 0, 0], [3, 4, 0]])
__X_B = np.array([[0, 0, 1], [3, 1, 0]])

__K = minmax_kernel(__X_A)
np.testing.assert_array_equal(np.diag(__K), np.ones((3,)))
np.testing.assert_equal(__K.shape, (3, 3))
assert(np.max(__K) <= 1.), "Kernel values must be <= 1"
assert(np.min(__K) >= 0.), "Kernel values must be >= 0"
np.testing.assert_equal(__K[0, 1], 0.)
np.testing.assert_equal(__K[1, 0], 0.)
np.testing.assert_equal(__K[0, 2], 1. / 9.)
np.testing.assert_equal(__K[2, 0], 1. / 9.)
np.testing.assert_equal(__K[1, 2], 1. / 7.)
np.testing.assert_equal(__K[2, 1], 1. / 7.)

__K = minmax_kernel(__X_A, __X_B)
np.testing.assert_equal(__K.shape, (3, 2))
assert(np.max(__K) <= 1.), "Kernel values must be <= 1"
assert(np.min(__K) >= 0.), "Kernel values must be >= 0"
np.testing.assert_equal(__K[0, 1], 1. / 6.)
np.testing.assert_equal(__K[1, 0], 0.)
np.testing.assert_equal(__K[1, 1], 1. / 4.)
np.testing.assert_equal(__K[2, 1], 4. / 7.)
```

1.3 3. Toxicity Prediction using Non-Linear SVMs (1 Bonus Point)

In this task you will predict whether a molecule can bind to a given receptor in the human body or not. Such prediction tasks do have relevance for drug design or environmental polution research. You are given a dataset with 600 molecular structures represented as molecular counting fingerprints (compare exercise 2), i.e. a non-negative vector where each entry counts the occurance of a predefined substructure in a molecule:



Let in the following $c(m_i) \in \mathbb{N}_0^d$ be the count vector representation of the molecule m_i. Furthermore, let $b(m_i) \in \{0,1\}^d$ its binary representation, i.e. $b(m_i)_s = \begin{cases} 1 & \text{if } c(m_i)_s > 0 \\ 0 & \text{else} \end{cases}$. Depending on the kernel function we use, we define $\mathbf{x}_i = c(m_i)$ respectively $\mathbf{x}_i = b(m_i)$

For each molecule you have the label $y_i \in \{-1, 1\}$ whether or whether not the molecules binds with the aryl hydrocarbon receptor.

[222]:
```
def read_tox_data(idir="/coursedata/", balance_classes=True,
                  random_state=211, n_samples=600):
    """
    Read in toxicity dataset.
    """
    smi_X = np.genfromtxt(idir + "/maccs_count_nrahr.csv", delimiter=",",␣
↪comments=None, usecols=(0,), dtype="str")
    smi_y = np.genfromtxt(idir + "/tox_nrahr.csv", delimiter=",",␣
↪comments=None, usecols=(0,), dtype="str")

    X = np.genfromtxt(idir + "/maccs_count_nrahr.csv", delimiter=",",␣
↪comments=None)[:, 1:]
    y = np.genfromtxt(idir + "/tox_nrahr.csv", delimiter=",", usecols=(1,),␣
↪comments=None, dtype="int")
    y[y == 0] = -1

    assert(np.all(smi_X == smi_y))
    assert(len(np.unique(smi_X)) == len(smi_X))

    if balance_classes:
        n_neg, n_pos = np.sum(y == -1), np.sum(y == 1)
        idc_neg = np.random.RandomState(random_state).choice(n_neg, n_pos,␣
↪replace=False)

        X_pos = X[y == 1]
        X_neg = X[y == -1][idc_neg]
```

```
        y_pos = y[y == 1]
        y_neg = y[y == -1][idc_neg]

        X, y = np.concatenate((X_pos, X_neg)), np.concatenate((y_pos, y_neg))

    # Get a random set of samples
    rng = np.random.RandomState(random_state)
    rnd_idx = rng.choice(X.shape[0], n_samples, replace=False)

    return X[rnd_idx], y[rnd_idx]
```

[223]:
```
# Read in data
X, y = read_tox_data()

# Split into train and test
X_train_c, X_test_c, y_train, y_test = train_test_split(X, y, random_state=3211)

# Create binary version of count vector
X_train_b, X_test_b = (X_train_c > 0).astype("float"), (X_test_c > 0).
↪astype("float")
```

Tasks:

- Compare the performance of the Gaussian (rbf)-, MinMax- and Tanimoto Kernel (previous task) using on a test set.
- Optimize the SVM hyper-parameters (and Gaussian-kernel parameters) using grid-search and 3-fold cross-validation.
- Make use of the sklearn C-SVM (imported as `SVM_sk`) implementation (due to faster optimization).

Hints / Notes:

- In this application the MinMax-kernel (for counting data) performs the best.
- In the sklearn package, the gaussian kernel is called RBF-kernel and its parameter is γ.

[227]:
```
X_train_c.shape
```

[227]:
```
(450, 142)
```

[231]:
```
y_train.shape
```

[231]:
```
(450,)
```

[243]:
```
from sklearn.model_selection import GridSearchCV
# Define the range of the hyper-parameters for the grid-search
C_range = 2.**np.arange(-2, 5)
gamma_range = np.array([0.001, 0.01, 0.1, 1.])

# Define the random states for the cross-validation
```

```
random_state_cv = 10909  # do not change!

# Define a 3-fold cross-validation using the sklearn
cv = KFold(n_splits=3, random_state=random_state_cv, shuffle=True)
# YOUR CODE HERE
#raise NotImplementedError()
assert(cv.random_state == random_state_cv), "Set the KFold random state."

# Define 3 SVMs: using rbf-kernel, minmax-kernel and tanimoto kernel
svm_gaus, svm_mm, svm_tan = SVM_sk(kernel='rbf'), SVM_sk(kernel=minmax_kernel),␣
 ↪SVM_sk(kernel=tanimoto_kernel)


# Define 3 GridSearchCV objects using the different SVMs
est_gaus, est_mm, est_tan = None, None, None
# YOUR CODE HERE
est_gaus = GridSearchCV(svm_gaus, param_grid={'C':C_range, 'gamma':
 ↪gamma_range}, cv=cv)
est_mm = GridSearchCV(svm_mm, param_grid={'C':C_range}, cv=cv)
est_tan = GridSearchCV(svm_tan, param_grid={'C':C_range}, cv=cv)
#raise NotImplementedError()

# Fit the grid-search objects with the training data
# YOUR CODE HERE
est_gaus.fit(X_train_c, y_train)
print("gauss done")
est_mm.fit(X_train_c, y_train)
print("minmax done")
est_tan.fit(X_train_b, y_train)
print("tan done")
#raise NotImplementedError()

print("(RBF-kernel) score:", np.round(est_gaus.score(X_test_c, y_test), 2),
      "best params:", est_gaus.best_params_)
print("(MinMax-kernel) score:", np.round(est_mm.score(X_test_c, y_test), 2),
      "best params:", est_mm.best_params_)
print("(Tanimoto-kernel) score:", np.round(est_tan.score(X_test_b, y_test), 2),
      "best_params:", est_tan.best_params_)
```

```
gauss done
minmax done
tan done
(RBF-kernel) score: 0.78 best params: {'C': 2.0, 'gamma': 0.01}
(MinMax-kernel) score: 0.83 best params: {'C': 2.0}
(Tanimoto-kernel) score: 0.77 best_params: {'C': 4.0}
```

[ ]:

[ ]: