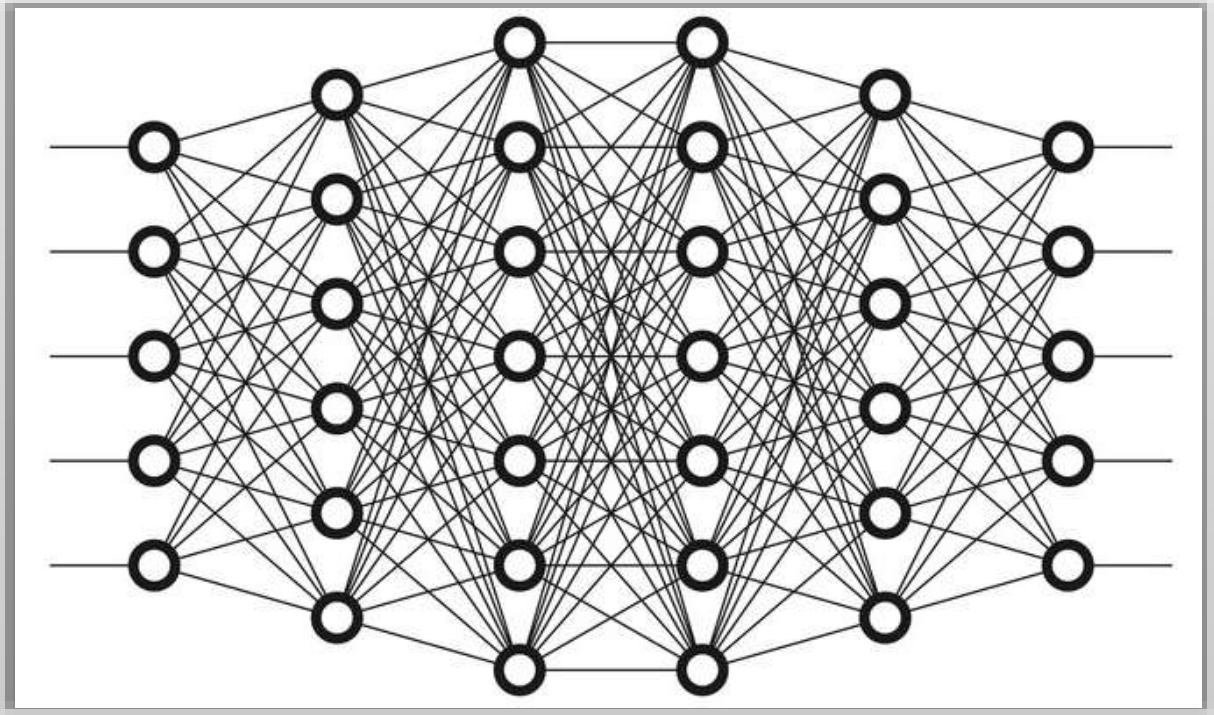
2023 年度云南大学软件学院本科生课程

机器学习实验

SVM与核方法

教 师： 李 劲（**lijin@ynu.edu.cn**）

2023 年 10 月



实验2. SVM与核方法

Kernel function

任务1. 实现三个核函数，并通过函数图像分析核函数性质

- **Linear kernel (**linear_kernel**) :** $k(\mathbf{x}, \mathbf{z}) = \sum_{f=1}^{F} x_f z_f = \mathbf{x}^\top \mathbf{z}$
- **polynomial kernel (**poly_kernel**) :** $k(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^\top \mathbf{z} + c)^p$
- **Gaussian kernel (**sqexp_kernel**) :** $k(\mathbf{x}, \mathbf{z}) = \exp\left(-\frac{(\mathbf{x}-\mathbf{z})^\top(\mathbf{x}-\mathbf{z})}{\ell^2}\right) = \exp\left(-\frac{\sum_{f=1}^{F}\left(x_f - z_f\right)^2}{\ell^2}\right)$
- **Periodic kernel (**periodic_kernel**) :** $k(\mathbf{x}, \mathbf{z}) = \exp\left(-\frac{1}{2}\frac{\left(\sin\left(\frac{\pi}{p}(\mathbf{x}-\mathbf{z})\right)\right)^2}{\ell^2}\right)$
- RBF核$k(\mathbf{x}, \mathbf{z}) = \alpha \exp\left(-\gamma(\mathbf{x}-\mathbf{z})^\top(\mathbf{x}-\mathbf{z})\right)$

1.1 基于python和numpy实现5个核函数（kernel function）.

1.2 对于上述5个核函数，分别绘制出两个函数: $k(x,1)$， $k(x,0)$的图像

1.3 对于poly_kernel, GK,PeriodicK，RBF核，通过绘制不同超参数的$k(x,1)$， $k(x,0)$ （ $x \in [-6,6]$ ）的图像，并分析超参数ℓ， p，α，γ对于上述核函数的影响，得出具体结论。

Kernel function

```
def  linear_kernel(x_QF, x_train_NF=None):
    ''' Evaluate linear kernel matrix between two datasets.

    Will compute the kernel function for all possible pairs of feature vectors,
    one from the query dataset, one from the reference training dataset.

                Args
                ----
    x_QF : 2D numpy array, shape (Q, F) = (n_query_examples, n_features)
                            Feature array for *query* dataset
                            Each row corresponds to the feature vector on example

    x_train_NF : 2D numpy array, shape (N, F) = (n_train_examples, n_features)
                            Feature array for reference *training* dataset
                            Each row corresponds to the feature vector on example

    Returns
    -------
    k_QN : 2D numpy array, shape (Q, N)
       Entry at index (q,n) corresponds to the kernel function evaluated
       at the feature vectors x_QF[q] and x_train_NF[n]
    '''
```

```
>>> np.set_printoptions(precision=3, suppress=1)

# Kernel evaluations with F=1 features
>>> x_zero_11 = np.asarray([[0.0]])
>>> x_one_11 = np.asarray([[1.0]])

# Linear kernel k(0,0) should be zero
>>> k_11 = calc_linear_kernel(x_zero_11, x_zero_11)
>>> k_11.ndim
2
>>> k_11
array([[0.]])

# Linear kernel k(1,1) should be one
>>> calc_linear_kernel(x_one_11, x_one_11)
array([[1.]])

# Linear kernel k(1, 3.456) should be 3.456
>>> calc_linear_kernel(x_one_11, 3.456 * x_one_11)
array([[3.456]])


# Part 2: Kernel evaluations with F=2 features and several examples at once
>>> x_train_32 = np.asarray([[0.0, 0.0], [1.0, 1.0], [2.0, 2.0]])
>>> calc_linear_kernel(x_train_32, x_train_32)
array([[0., 0., 0.],
       [0., 2., 4.],
       [0., 4., 8.]])
```

Kernel function

```
def sqexp_kernel(x_QF, x_train_NF=None, length_scale=1.0):
    ''' Evaluate squared-exponential kernel matrix between two datasets.
    Will compute the kernel function for all possible pairs of feature vectors,
    one from the query dataset, one from the reference training dataset.
    Args
                ----
    x_QF : 2D numpy array, shape (Q, F) = (n_query_examples, n_features)
                            Feature array for *query* dataset
                            Each row corresponds to the feature vector on example

    x_train_NF : 2D numpy array, shape (N, F) = (n_train_examples, n_features)
                            Feature array for reference *training* dataset
                            Each row corresponds to the feature vector on example

    Returns
    -------
    k_QN : 2D numpy array, shape (Q, N)
       Entry at index (q,n) corresponds to the kernel function evaluated
       at the feature vectors x_QF[q] and x_train_NF[n]
    '''
```

```
>>> np.set_printoptions(precision=3, suppress=1)

# Example 1: Simple kernel evaluations with F=1 features
>>> x_zero_11 = np.asarray([[0.0]])
>>> x_one_11 = np.asarray([[1.0]])
>>> k_11 = sqexp_kernel(x_zero_11, x_zero_11, length_scale=1.0)
>>> k_11.ndim
2
>>> k_11
array([[1.]])
>>> sqexp_kernel(x_one_11, x_one_11, length_scale=1.0)
array([[1.]])
>>> sqexp_kernel(x_one_11, x_zero_11, length_scale=1.0)
array([[0.368]])


# Example 2: Kernel evaluations with F=2 features and several examples at once
>>> x_train_32 = np.asarray([[0.0, 0.0], [1.0, 1.0], [2.0, 2.0]])
>>> k_33 = sqexp_kernel(x_train_32, x_train_32)
>>> k_33
array([[1.   , 0.135, 0.   ],
       [0.135, 1.   , 0.135],
       [0.   , 0.135, 1.   ]])
```

Kernel function

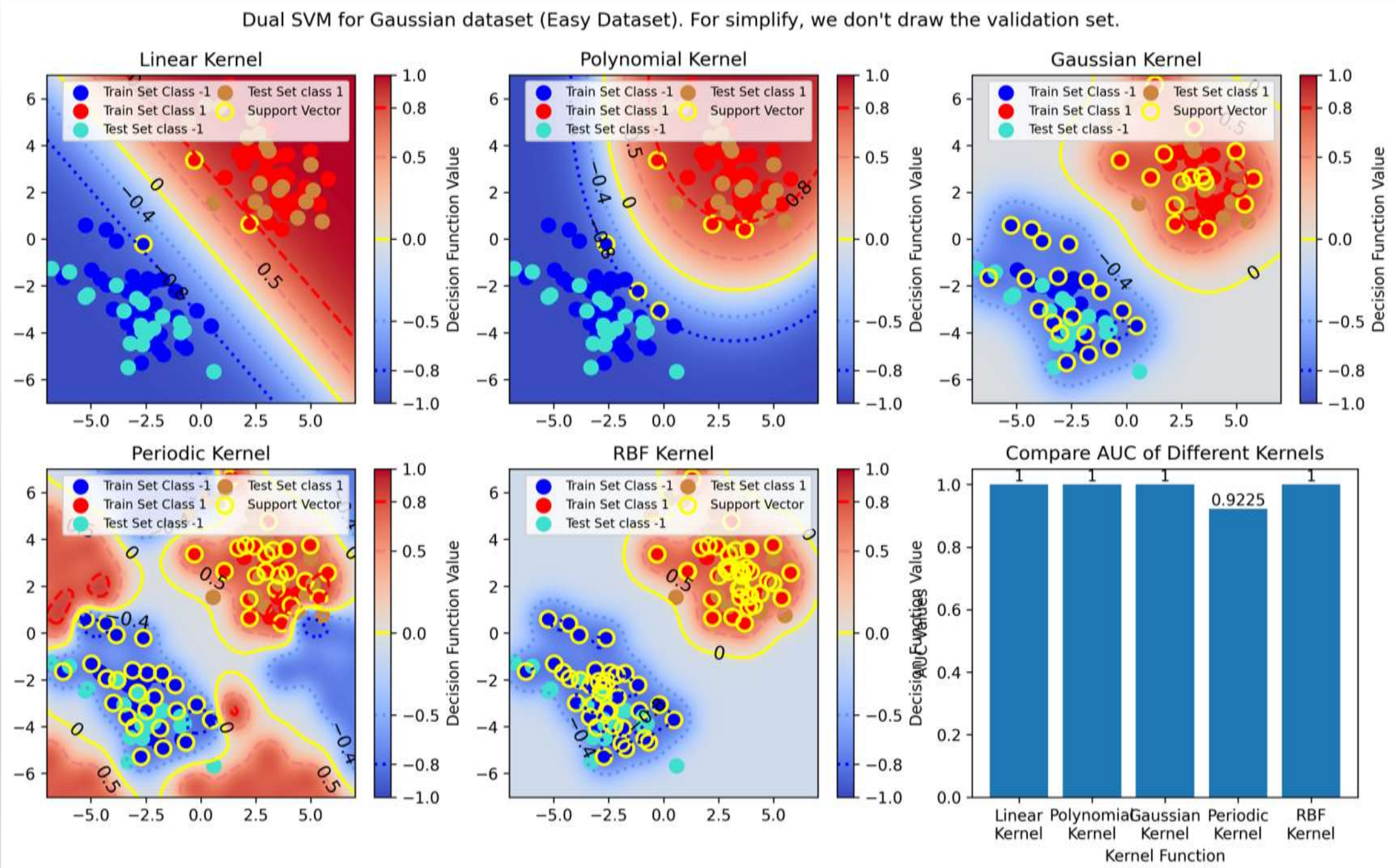
```
def periodic_kernel(x_QF, x_train_NF=None, length_scale=1.0, period=1.0):
    ''' Evaluate periodic kernel to produce matrix between two datasets.

    Will compute the kernel function for all possible pairs of feature vectors,
    one from the query dataset, one from the reference training dataset.

    Args
    ----
    x_QF : 2D numpy array, shape (Q, F) = (n_query_examples, n_features)
        Feature array for *query* dataset
        Each row corresponds to the feature vector on example

    x_train_NF : 2D numpy array, shape (N, F) = (n_train_examples, n_features)
        Feature array for reference *training* dataset
        Each row corresponds to the feature vector on example

    Returns
    -------
    k_QN : 2D numpy array, shape (Q, N)
        Entry at index (q,n) corresponds to the kernel function evaluated
        at the feature vectors x_QF[q] and x_train_NF[n]
    '''
```

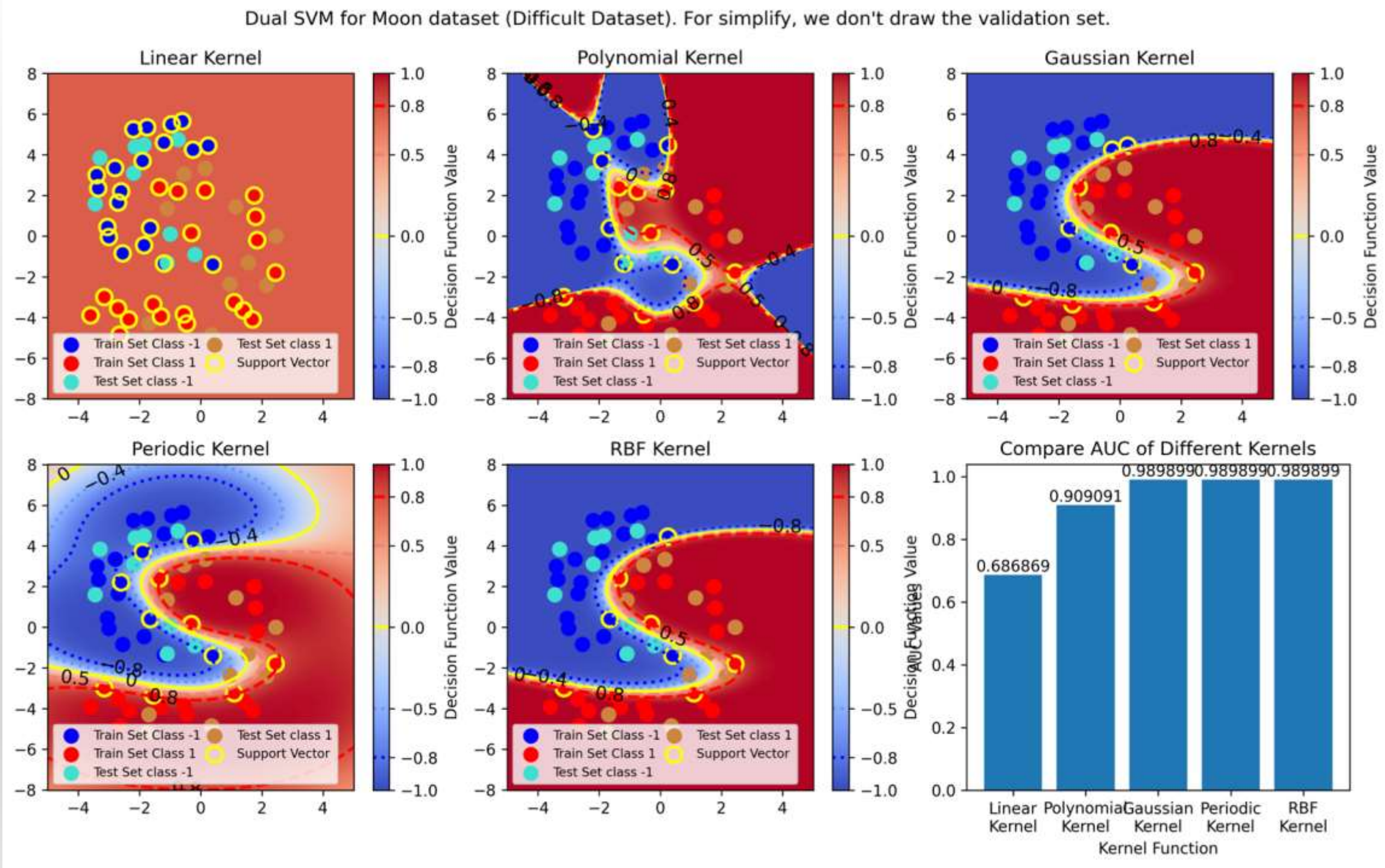
```
Examples
--------
>>> np.set_printoptions(precision=3, suppress=1)

# Part 1: Simple kernel evaluations with F=1 features
>>> x_zero_11 = np.asarray([[0.0]])
>>> x_one_11 = np.asarray([[1.0]])

# Kernel of x=0.0 with itself should be 1.0
>>> k_11 = periodic_kernel(x_zero_11, x_zero_11, length_scale=2.0, period=0.3)
>>> k_11.ndim
2
>>> k_11
array([[1.]])

# Kernel of x and z=x+period should be 1.0
>>> p = 0.3
>>> periodic_kernel(x_one_11, x_one_11 + p, length_scale=2.0, period=p)
array([[1.]])
>>> periodic_kernel(x_one_11, x_one_11 + 3 * p, length_scale=2.0, period=p)
array([[1.]])

# Part 2: Kernel evaluations with several examples at once (still F=1)
>>> x_train_31 = np.asarray([[0.0], [1.0], [2.0]])
>>> periodic_kernel(x_train_31, x_train_31, length_scale=2.0, period=0.95)
array([[1.   , 0.997, 0.987],
       [0.997, 1.   , 0.997],
       [0.987, 0.997, 1.   ]])
>>> x_test_21 = np.asarray([[-0.5], [0.5]])
>>> periodic_kernel(x_test_21, x_train_31, length_scale=2.0, period=0.95)
array([[0.883, 0.889, 0.9  ],
       [0.883, 0.883, 0.889]])
```

Kernel SVM

任务2. 生成和读入两个数据集（分别称为Gaussian， Moon）. 其中， Gaussian在二维平面上分别以 $X_1 \sim N\left([-3,-3],\begin{bmatrix}2,-1\\-1,2\end{bmatrix}\right)$, $X_2 \sim N\left([3,3],\begin{bmatrix}2,-1\\-1,2\end{bmatrix}\right)$ 各随机生成80个样本点（ X_1 样本点作为-1类， X_2 样本点作为+1类），按照40:20:20划分为“训练集”、“验证集”、“测试集”，并绘制。Moon数据集由Moon.txt提供。

任务3. 基于python和numpy，以及cvxopt（cvxopt.org **）设计并实现核SVM模型 (需自己实现，不允许直接调用已有库中SVM的实现). 分别利用linear_kernel 、 ploy_kernel 、 sqexp_kernel 、periodic_kernel、 rbf_kernel实现上述不同的核SVM模型。并用“训练集”进行模型训练；基于“验证集”用grid search（Scikit-Learn GridSearchCV）方法选择核函数中最优超参数；最后，在测试集上进行模型验证，给出不同核回归模型的AUC分类对比结果，并对该结果进行分析。对于不同的核SVM模型，绘制“训练集”“测试集”，并绘制分类曲线、间隔曲线以及标识出支持向量**


Dual SVM for Gaussian dataset (Easy Dataset). For simplify, we don't draw the validation set.
Linear Kernel
Polynomial Kernel
Gaussian Kernel
Periodic Kernel
RBF Kernel
Compare AUC of Different Kernels
Train Set Class -1
Train Set Class 1
Test Set class -1
Test Set class 1
Support Vector
Decision Function Value
AUC Values
Kernel Function
Linear Kernel
Polynomial Kernel
Gaussian Kernel
Periodic Kernel
RBF Kernel
1
1
1
0.9225
1


Dual SVM for Moon dataset (Difficult Dataset). For simplify, we don't draw the validation set.
Linear Kernel
Polynomial Kernel
Gaussian Kernel
Periodic Kernel
RBF Kernel
Compare AUC of Different Kernels
Train Set Class -1
Train Set Class 1
Test Set class -1
Test Set class 1
Support Vector
Decision Function Value
AUC Values
0.686869
0.909091
0.9898990.9898990.989899
Linear Kernel
Polynomial Kernel
Gaussian Kernel
Periodic Kernel
RBF Kernel
Kernel Function