ML_HW5_report

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- I. Gaussian Process
 - A. code with detailed explanations (20%)
 - 1. Part1: Apply Gaussian Process Regression to predict the distribution of *f* and visualize the result.
 - a) Running command:\$ python3 main.py hw5-1
 - b) read input data(in main.py): I use np.genfromtxt to read the input data as np.ndarray and pass input data into my implement function gaussianProcessRegression(), which is defined in ml/Gaussian_process.py.

```
if (sys.argv[1] == 'hw5-1'):
    if (len(sys.argv) != 2):
        usage()
    # read data
    input_data = np.genfromtxt('./data/input.data', delimiter=' ')
    ml.gaussianProcessRegression(input_data)
```

c) Rational Quadratic Kernel(Gaussian_process.py) Rational Quadratic Kernel is parameterized by a length scale parameter l>0 and a scale mixture parameter a>0. The kernel is given by:

$$k(x_i,x_j) = \left(1 + rac{d(x_i,x_j)^2}{2lpha l^2}
ight)^{-lpha}$$

, where α is the scale mixture parameter, l is the length scale of the kernel and $d(\cdot, \cdot)$ is the

Euclidean distance.

I implement it in the rationalQuadraticKernel() function and set default length = 1 and alpha = 1.

d) computeGaussianProcess(): compute Gaussian Process and do prediction, it return $\mu(x^*)$ and $\sigma^2(x^*)$.

First, we want to compute the marginal likelihood P(y) = N(y|0, C), where the covariance matrix C has elements

$$\mathbf{C}(\mathbf{x}_n, \mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m) + \beta^{-1} \delta_{nm}$$

Thus, we compute covariance matrix C as follows

```
# Gaussian process regression
# k(x, x)
k_x_x = rationalQuadraticKernel(X, X, length, alpha)
# covariance matrix
C = k_x_x + (1 / beta) * np.identity(X.shape[0])
```

Next, we want to predict the distribution of new f^* , we just need to cut the covariance matrix C on f^* to see the conditional distribution thus achieve prediction.

conditional distribution $p(y^*|y)$ is a Gaussian distribution with:

$$\mu(\mathbf{x}^*) = k(\mathbf{x}, \mathbf{x}^*)^{\top} \mathbf{C}^{-1} \mathbf{y}$$

$$\sigma^2(\mathbf{x}^*) = k^* - k(\mathbf{x}, \mathbf{x}^*)^{\top} \mathbf{C}^{-1} k(\mathbf{x}, \mathbf{x}^*)$$

$$k^* = k(\mathbf{x}^*, \mathbf{x}^*) + \beta^{-1}$$

following the above formula, the code is:

e) Visualize: Finally, i use matplotlib.pyplot to visualize the result of Gaussian Process Regression. The 95% confidence interval indicates that the Z score is 1.96. And the Z score formula is: $z=\frac{x-\mu}{\sigma}$, thus we get the confidence interval is

```
# 95% confidence interval = 1.96x variance
confidence_interval_95 = 1.96 * var
```

Then, we can draw the figure by following code

```
drawRegression(X_star[:, 0], predict_mean[:, 0], confidence_interval_95)

def drawRegression(x, y, boundary):
    plt.plot(x, y, linewidth=1, color='blue')
    plt.plot(x, y + boundary, linewidth=1, color='red')
    plt.plot(x, y - boundary, linewidth=1, color='red')
    plt.fill_between(x, y + boundary, y - boundary, color='coral', alpha=0.5)
    plt.xlim(-60.0, 60.0)
    plt.ylim(-3.0, 3.0)
```

- 2. Part2: Optimize the kernel parameters by minimizing negative marginal log-likelihood, and visualize the result again.
 - a) Optimize the kernel parameters: According to our kernel function, we have two parameters need to be optimized(length and alpha). In the beginning, I guess theta is(length = 1, alpha = 1), and I use scipy.optimize.minimize to optimize the

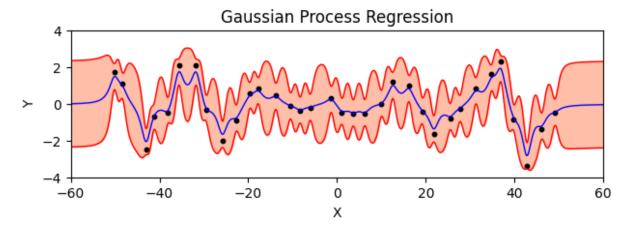
parameters(implement at the function optimizeKernelParameter()). I pass my compute negative marginal log likelihood function and theta to minimize and get optimized parameters.

```
opt_result = minimize(
    computeNegativeMarginalLogLikelihood,
    theta,
    args=(
        X,
        Y,
        beta))
```

b) compute negative marginal log likelihood: First, we use rationalQuadraticKernel() to get covariance matrix C_{θ} . The marginal likelihood function is $p(y|\theta) = N(y|0, C_{\theta})$. Thus, the negative marginal log likelihood is $-\ln p(y|\theta) = \frac{1}{2} \ln |C_{\theta}| + \frac{1}{2} y^T C_{\theta}^{-1} y + \frac{N}{2} \ln (2\pi)$ According to above formula, the code implement is

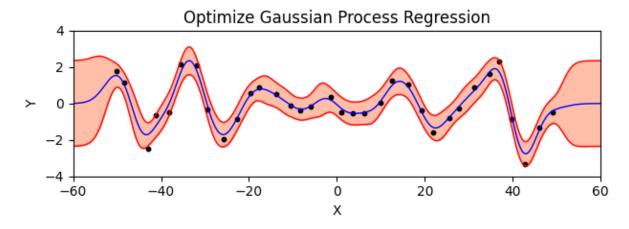
- c) Visualize: same as part1.
- B. experiments settings and results
 - 1. Part1:

$$l = 1$$
, $\alpha = 1$



2. Part2:

$$l = 2.9679647$$
, $\alpha = 473.616351$



C. observations and discussion

- 1. The optimized version is better than the original version.
- 2. The bigger length² is, the less wiggly your random functions are. This is because larger length will effectively be blurring together points in a larger window. Thus, you can see the wiggly in the optimized version(l = 2.9679647) is less than the original version (l = 1).
- 3. The 95% confidence interval of the optimized version is smaller than the original version.
- 4. The interval with data points has a smaller confidence interval than the interval without data points. This means the interval with data points is easier to predict than the interval without data points.
- 5. Using default parameters (l = 1, $\alpha = 1$) is about 2.3 times faster than using optimized parameters (l = 2.9679647, $\alpha = 473.616351$).

II. SVM

- A. code with detailed explanations (20%)
 - 1. Part1: Use different kernel functions (linear, polynomial, and RBF kernels) and compare their performance.
 - a) Running command:\$ python3 main.py hw5-2
 - b) Read data in main.py: I directly read data in the ./data/*.csv and pass data into my implement

function ml.SVM(), which is defined in ml/SVM.py.

```
elif (sys.argv[1] == 'hw5-2'):
    if (len(sys.argv) != 2):
        usage()
    # read data
    X_train = np.genfromtxt('./data/X_train.csv', delimiter=',')
    Y_train = np.genfromtxt('./data/Y_train.csv', delimiter=',')
    X_test = np.genfromtxt('./data/X_test.csv', delimiter=',')
    Y_test = np.genfromtxt('./data/Y_test.csv', delimiter=',')
    Y_test = np.genfromtxt('./data/Y_test.csv', delimiter=',')
    Ml.SVM(X_train, Y_train, X_test, Y_test)
```

c) At SVM.py: Since I need to compare the performance of three kernel functions, I call my own function computeSVMAndTime() to compute SVM and measure the execution time.

```
print('===== Compare the performance with linear, polynomial, RBF kernel function ======')
# linear = 0
computeSVMAndTime(0, X_train, Y_train, X_test, Y_test)
# polynomial = 1
computeSVMAndTime(1, X_train, Y_train, X_test, Y_test)
# radial basis function(RBF) = 2
computeSVMAndTime(2, X_train, Y_train, X_test, Y_test)
```

d) computeSVMAndTime(): I use the option -t provided in the libsvm package to indicate the kernel function I want. The number 0 represents linear, 1 represents polynomial and 2 represents RBF. I pass the kernel_type by the first parameter and call the svm_train for training the model. Finally, I call svm_predict to use my model to predict the test data. I compute the training and prediction time and print the total execution time in the end. (The code is pasted on the next page.)

- 2. Part2: Please do the grid search for finding parameters of the best performing model.
 - a) I tried to find the best parameters for all kernel functions. Thus, I call the function gridSearch() three times by passing different kernel function types.

```
print('\n===== Use grid search method to find the best performing parameters in each kernel function ======')
# linear = 0
gridSearch(0, X_train, Y_train)
# polynomial = 1
gridSearch(1, X_train, Y_train)
# radial basis function(RBF) = 2
gridSearch(2, X train, Y train)
```

b) The formula of the three kernel functions: Since we want to find out the best parameters of each kernel function, we need to figure out the formula of each kernel function first.

```
linear kernel: k(u, v) = \langle u, v \rangle

polynomial kernel: k(u, v) = (\gamma * \langle u, v \rangle + coef 0)^d

RBF kernel: k(u, v) = e^{-\gamma ||u-v||^2}
```

Because in C-SCV, all kernel functions have a parameter C. Therefore, the parameters that need to be trained for each kernel function are summarized in the below table.

kernel function	linear	polynomial	RBF
need parameters	С	c, γ, coef0, d	<i>c</i> , γ

The below table is the parameters I am trying to tune.

parameters	С	γ	coef0	d
tuning value	0.1, 1, 10	$\frac{1}{784}$, 0.1, 0	0.1, 1, 10	0, 1, 2, 3

```
cost = [np.power(10.0, i) for i in range(-1, 2)]
gamma = [1.0 / 784] + [np.power(10.0, i) for i in range(-1, 1)]
coef0 = [np.power(10.0, i) for i in range(-1, 2)]
degree = [i for i in range(0, 4)]
```

Since we need to do cross-validation, we should decide the number of n fold we use. There, I set n=3 in my implementation.

```
# set n fold
num_n = 3
```

Then I tried all possible combinations of parameters and found out the best accuracy and best parameters in each kernel function. Finally, I use the best parameters to train the model and make predictions.

Paste the complete code as follows:

gridSearch(): which implements the grid search.

```
| kernel_type: int, | X_train: np.ndarray, | Y_train: np.ndarray, | Y_train: np.ndarray, | Y_train: np.ndarray, | X_train: np.ndarray, |
```

Linear:

```
if kernel_type == 0:
   print('kernel function: linear')
   cost = [np.power(10.0, i) for i in range(-1, 2)]
   save_stdout = sys.stdout
   sys.stdout = open(os.devnull, 'w')
        parameters = svm_parameter(
            str(kernel_type) +
            str(num_n) +
            ' -q')
       problem = svm_problem(Y_train, X_train)
       accuracy = svm_train(problem, parameters)
        if accuracy > best_accuracy:
           best_accuracy = accuracy
           best parameter = {'cost': c}
   sys.stdout = save_stdout
   opt_parameters = svm_parameter(
        '-t ' + str(kernel_type) + ' -c ' + str(best_parameter['cost']) + ' -q')
   problem = svm problem(Y train, X train)
   model = svm_train(problem, opt_parameters)
   p_label, p_acc, p_val = svm_predict(Y_test, X_test, model)
```

plynomial:

```
elif kernel_type == 1:
   print('kernel function: polynomial')
    cost = [np.power(10.0, i) for i in range(-1, 2)]
    gamma = [1.0 / 784] + [np.power(10.0, i) for i in range(-1, 1)]
    coef0 = [np.power(10.0, i) for i in range(-1, 2)]
   degree = [i \text{ for } i \text{ in } range(0, 4)]
    save_stdout = sys.stdout
    sys.stdout = open(os.devnull, 'w')
    for c in cost:
        for g in gamma:
            for r in coef0:
                for d in degree:
                    parameters = svm_parameter(
                        str(kernel_type) +
                        str(c) +
                        str(g) +
                        str(r) +
                        str(d) +
                        str(num n) +
                        ' -q')
                    problem = svm_problem(Y_train, X_train)
                    accuracy = svm_train(problem, parameters)
                    if accuracy > best_accuracy:
                        best_accuracy = accuracy
                        best_parameter = {
                            'cost': c, 'gamma': g, 'coef0': r, 'degree': d}
     sys.stdout = save stdout
     opt_parameters = svm_parameter('-t ' +
                                       str(kernel type) +
                                       str(best_parameter['cost']) +
                                        ' -a ' +
                                       str(best_parameter['gamma']) +
                                       str(best_parameter['coef0']) +
                                        ' -d ' +
                                       str(best_parameter['degree']) +
                                        ' -q')
     problem = svm_problem(Y_train, X_train)
     model = svm_train(problem, opt_parameters)
     p_label, p_acc, p_val = svm_predict(Y_test, X_test, model)
```

RBF:

```
elif kernel_type == 2:
    print('kernel function: RBF')
    cost = [np.power(10.0, i) for i in range(-1, 2)]
    gamma = [1.0 / 784] + [np.power(10.0, i) for i in range(-1, 1)]
   save stdout = sys.stdout
    sys.stdout = open(os.devnull, 'w')
    for c in cost:
        for g in gamma:
            parameters = svm_parameter(
                str(kernel type) +
                str(c) +
                str(g) +
                str(num_n) +
                ' -q')
            problem = svm problem(Y train, X train)
            accuracy = svm_train(problem, parameters)
            if accuracy > best_accuracy:
                best accuracy = accuracy
                best_parameter = {'cost': c, 'gamma': g}
    sys.stdout = save stdout
    opt parameters = svm parameter('-t ' +
                                    str(kernel type) +
                                    str(best_parameter['cost']) +
                                    ' -q ' +
                                    str(best parameter['gamma']) +
                                    ' -q')
    problem = svm_problem(Y_train, X_train)
    model = svm_train(problem, opt_parameters)
    p_label, p_acc, p_val = svm_predict(Y_test, X_test, model)
else:
    print('Invalid kernel_type[0 ~ 2], exit')
```

printGridSearchResult(best_accuracy, best_parameter)

exit(-1)

Finally, I call the function printGridSearchResult() to show the result.

```
def printGridSearchResult(best_accuracy: float, best_parameter: dict):
    print(f'Best performing accuracy: {best_accuracy:.2f}%')
    print(f'Best parameters: {best_parameter}\n')
```

- 3. Part3: Use linear kernel + RBF kernel together (therefore a new kernel function) and compare its performance with respect to others.
 - a) User defined kernel in libsvm: First of all, we need to figure out how to use user-defined kernel function in libsvm. The option -t can set kernel function type and libsvm has provided some regular kernel functions(which used at previous implementation). Setting the option -t to value 4 means we use a precomputed kernel. If we set the option -t to value 4, then the training data of X(X_train) must rewrite to the following format:

index of X	return value of kernel function
1	k(1)
2	k(2)
n	k(n)

When passing our new data to svm_problem, we need to set the parameter 'isKernel=True' means that we use the kernel function that is defined by myself. The code show as below:

b) Code implement:

First, I defined my own function to compute the linear and RBF kernel function.

Second, in the main implement function combineLinearAndRBF(), I tried to find out the best parameters(c and γ). Therefore, I use a grid search method with n=3 fold to find out the best accuracy model.

```
def combineLinearAndRBF(
       X_train: np.ndarray,
        Y_train: np.ndarray,
       X_test: np.ndarray,
       Y_test: np.ndarray):
   linear = computeLinearKernel(X_train, X_train)
   num_n = 3
   cost = [np.power(10.0, i) for i in range(-1, 2)]
   gamma = [1.0 / 784] + [np.power(10.0, i) for i in range(-1, 1)]
   best_accuracy = 0
   best_gamma = 0
   train_rows = X_train.shape[0]
   save_stdout = sys.stdout
       for g in gamma:
            rbf = computeRBF(X_train, X_train, g)
                (np.arange(1, train_rows + 1).reshape(-1, 1), linear + rbf))
            parameters = svm_parameter(f'-t 4 -c {c} -v {num_n} -q')
            problem = svm_problem(Y_train, combination, isKernel=True)
            accuracy = svm_train(problem, parameters)
            if accuracy > best_accuracy:
                best_accuracy = accuracy
                best_c = c
                best_gamma = g
```

Finally, I put the best parameters I searched before in the parameters to train the model. Then I transform the X_test data form and predict the X_test data. Measuring the execution time starts from the training model and ends after finishing prediction.

```
best_gamma = g
start_time = time.time()
rbf = computeRBF(X_train, X_train, best_gamma)
combination = np.hstack(
    (np.arange(1, train_rows + 1).reshape(-1, 1), linear + rbf))
parameters = svm_parameter(f'-t 4 -c {best_c} -q')
problem = svm_problem(Y_train, combination, isKernel=True)
model = svm_train(problem, parameters)
sys.stdout = save_stdout
print(f'Combine linear and RBF kernel function')
print(f'Best accuracy: {best_accuracy}%')
print(f'Best parameters: cost = {best_c}, gamma = {best_gamma}')
test rows = X test.shape[0]
linear = computeLinearKernel(X_test, X_test)
rbf = computeRBF(X_test, X_test, best_gamma)
new_X_test = np.hstack(
    (np.arange(1, test_rows + 1).reshape(-1, 1), linear + rbf))
p_label, p_acc, p_val = svm_predict(Y_test, new_X_test, model)
print(f'Predict accuracy: {p_acc}%')
end_time = time.time()
print(f'total cost {end_time - start_time:.2f} sec.\n')
```

B. experiments settings and results (20%)

1. Part1:

```
==== Compare the performance with linear, polynomial, RBF kernel function =====
kernel_type: linear
Accuracy = 95.08% (2377/2500) (classification)
train cost 1.52660 sec.
predict cost 1.04186 sec.
total cost 2.57 sec.
kernel type: polynomial
Accuracy = 34.68\% (867/2500) (classification)
train cost 18.87900 sec.
predict cost 6.21107 sec.
total cost 25.09 sec.
kernel_type: RBF
Accuracy = 95.32% (2383/2500) (classification)
train cost 3.42083 sec.
predict cost 2.21455 sec.
total cost 5.64 sec.
```

2. Part2:

```
===== Use grid search method to find the best performing parameters in each kernel function kernel function: linear

Accuracy = 95.8% (2395/2500) (classification)

Best performing accuracy: 96.66%

Best parameters: {'cost': 0.1}

kernel function: polynomial

Accuracy = 97.84% (2446/2500) (classification)

Best performing accuracy: 98.16%

Best parameters: {'cost': 0.1, 'gamma': 1.0, 'coef0': 10.0, 'degree': 2}

kernel function: RBF

Accuracy = 96.28% (2407/2500) (classification)

Best performing accuracy: 97.24%

Best parameters: {'cost': 10.0, 'gamma': 0.0012755102040816326}
```

3. Part3: (compare by part1.)

```
===== Combine Linear and RBF kernel function and compare the performance with others Combine linear and RBF kernel function
Best accuracy: 96.82%
Best parameters: cost = 0.1, gamma = 0.1
Accuracy = 24.56% (614/2500) (classification)
train cost 19.77645 sec.
transform X_test cost 2.59439 sec.
predict cost 2.18856 sec.
total cost 24.56 sec.
```

- C. observations and discussion (10%)
 - 1. We can summarize the performance of each kernel function in the following table.

kernel function	linear	polynomial	RBF	linear+RBF
train time	1.52660	18.87900	3.42083	19.77645
transform time	X	X	X	2.59439
predict time	1.04186	6.21107	2.21455	2.18856
performance(sec)	2.57	25.09	5.64	24.56
predict accuracy (part1)	95.08%	34.68%	95.32%	Х
predict accuracy (part2)	95.8%	97.84%	96.28%	Х
best parameter (part2)	cost=0.1	cost=0.1 gamma=1 coef0=10 degree=2	cost=10 gamma $= \frac{1}{784}$	cost=0.1 gamma=0.1 (part3)
predict accuracy (part3)	X	X	X	24.56%

- 2. We can observe that the training took more time than predicted.
- 3. The observation is that the more parameters the kernel function uses, the more time cost in training the model and prediction.
 - (poly (4 param)>RBF (2 param)>linear(1 param))
- 4. The observation is that user defined kernel functions cost more times than original kernel functions in training stage.(19.16916 > 1.53887 + 3.41844)
- 5. Since the polynomial kernel function has four parameters, when executing the grid methods it costs more time than other kernel functions.
- 6. According to the result of part1 and part2, we can find that the RBF kernel function has higher predicted accuracy than others. This is because RBF can project

- data into an infinite dimension feature space, and it can find a hyperplane to better separate the data.
- 7. After using the grid search method, the accuracy of the polynomial kernel function increases the most (34.68% -> 97.84%).
- 8. The parameter cost C in C-SVM is a regularization parameter. This means how well the model tolerates outliers. The larger C we choose, the less outliers we can tolerate. Relatively, the larger C means the correctness of classify is higher.

Running environment:

```
python = "^3.8"
numpy = "^1.21"
scipy = "^1.6.1"
matplotlib = "^3.4"
pyqt5 = "^5.15"
numba = "^0.50"
libsvm-official = "^3.25"
```

Use poetry to build the environment and run the code:

- \$ poetry install --no-root
- \$ poetry shell
- \$ python3 main.py hw5-1 // hw5 part1
- \$ python3 main.py hw5-2 // hw5 part2