tags: Machine Learning

ML HW5: Gaussian Process and SVM

I. Gaussian Process

a. code with detailed explanations

- Part1
 - Kernel
 - The rational quadratic kernel I used is **Radial basis function kernel with** additional hyperparameter. The equation is:
 - $kernel = \sigma * exp(-\gamma ||x x'||_2^2)$
 - The additional parameter σ is used to scale the value of RBF kernel, trying to make it more flexible.

```
def kernel(X_M, X_N, sigma=1.0, gamma=1.0):
    """

kernel with quadratic term, linear term, and constant.

Args:
    X_M: Array of M values.
    X_N: Array of N values.
    sigma: hyper-parameter for RBF kernel.
    gamma: hyper-parameter for quadratic term.

Return Value:
    (M x N) matrix.
    """

MxN = np.matmul(X_M, np.transpose(X_N))
    RBF_k = sigma * np.exp((-1) * gamma * (X_M ** 2 + np.sum(X_N ** 2, axis=1) - 2 * MxN))
    return RBF_k
```

- Gaussian Process Regression and Prediction
 - In Gaussian Process, we need to construct three covariance matrices by kernel first. Each of them defines the following relations:
 - Covar: The relation between all training data points.
 - Covar_t: The relation between all training data points and all testing data points.
 - Covar_tt: The relation between all testing data points.
 - Then we can use the above covariance matrices, y value of training datas, and variance of noise to calculate the predictive means and variances since we know that the conditional distribution $p(y^*|y)$ is a Gaussian distribution with:
 - $ullet \mu(x^*) = k(x, x^*)^T * C_N^{-1} * y$
 - $\qquad \sigma^2(x^*) = k^* k(x, x^*)^T * C_N^{-1} * k(x, x^*)$
 - lacktriangledown where Covar = C_N , Covar_t = $k(x,x^*)$, and Covar_tt = k^* = $k(x^*,x^*)+eta^{-1}$

```
def prediction(Xtrain, Xtest, Ytrain, noise_var=1.0, sigma=1.0, gamma=1.0):
   Prediction by Gaussian Process Regression.
       Xtrain: Array of training data for X values. (M \times 1)
       Xtest: Array of testing data for X values.
       Ytrain: Array of training data for Y values. (M x 1)
       noise_var: Variance of noise.
       sigma, gamma: hyper-parameters for kernel.
   Return Value:
       mean: Array of mean values of each data in Xtest. (N x 1)
       variance: Array of variance values of each data in Xtest. (N x N)
   ## Covar: The relation between all training data points (M x M)
   ## Covar t: The relation between all training data points and all testing data points (M \times N)
   Covar = kernel(Xtrain, Xtrain, sigma, gamma) + noise_var * np.identity(Xtrain.shape[0])
   Covar_t = kernel(Xtrain, Xtest, sigma, gamma)
   Covar_tt = kernel(Xtest, Xtest, sigma, gamma) + noise_var * np.identity(Xtest.shape[0])
   Covar inv = np.linalg.inv(Covar)
   means = np.matmul(np.matmul(np.transpose(Covar_t), Covar_inv), Ytrain)
   variances = Covar_tt - np.matmul(np.matmul(np.transpose(Covar_t), Covar_inv), Covar_t)
   return means, variances
```

Train and Get Prediction

■ Use the default hyperparameters with Training data and Testing data to train a model, and get **the predictive means and variances**.

```
### Training and Prediction ###

noise_var = 1/5

Xtest = np.arange(start=-60, stop=60, step=0.1).reshape(-1, 1)

if Mode == 0:

sigma, gamma = 1.0, 1.0

means, variances = prediction(Xtrain, Xtest, Ytrain, noise_var, sigma, gamma)
```

Calculate 95% confidence interval

- The standard score for **95% confidence level** is **1.96**, and we can multiply it by **standard deviation** to get uncertain scale. Then we use it to calculate the **confidence limit** and get the **95% confidence interval**.
- The 95% CI for $\mu = \mu \pm 1.96 * \sigma$

```
CI = np.sqrt(np.diag(variances)) * 1.96

Xtest = Xtest.flatten()

means = means.flatten()

UpperBound, LowerBound = means + CI, means - CI
```

Visualization

I Use matplotlib.pyplot to mark the region of the confidence interval, predictive mean, and training data, so we can know how our model performs.

```
plt.plot(Xtest, means, color='blue')
plt.fill_between(Xtest, UpperBound, LowerBound, where= UpperBound >= LowerBound, \

facecolor = "yellow", edgecolor = "blue")

plt.plot(Xtrain, Ytrain, "o", color='green', markersize=5)

plt.title('hyperparam: \nsigma = {:.6f}, gamma = {:.6f}'.format(sigma, gamma))

plt.xlabel("X")
plt.ylabel("Y")

plt.xlim(-60, 60)

plt.show()
```

- Part2
 - Negative Marginal Log Likelihood

• We know that the marginal likelihood is a Gaussian distribution with mean = 0 and covariance = C.

$$\frac{1}{\sqrt{(2\pi)^k |\Sigma|}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1}(x-\mu)} = \frac{1}{\sqrt{(2\pi)^k |C|}} e^{-\frac{1}{2}(y-0)^T C^{-1}(y-0)}$$

■ In order to **optimize the hyperparameter of kernel**, we need to get the equation of **negative marginal log likelihood** and minimize it.

$$lacksquare -ln\ p(y| heta) = rac{1}{2}ln|C_ heta| + rac{k}{2}ln(2\pi) + rac{1}{2}y^TC_ heta^{-1}y$$

lacktriangle By computing the kernel, we can get the covariance C, which is the relation between all training data points.

```
def NegativeMarginalLogLikelihood(param, Xtrain, Ytrain, noise_var):
    """
    Calculate negative marginal log likelihood.
    Args:
        param: includes sigma, gamma, which are needed to optimize.
        Xtrain: Array of training data for X values. (M x 1)
        Ytrain: Array of training data for Y values. (M x 1)
        noise_var: Variance of noise.

Return Value:
        nmll: negative marginal log likelihood value for current parameter.

"""
sigma, gamma = param
    Covar = kernel(Xtrain, Xtrain, sigma, gamma) + noise_var * np.identity(Xtrain.shape[0])
    Covar_inv = np.linalg.inv(Covar)
    Ytrain_t = np.transpose(Ytrain)
    nmll = (1/2) * np.log(np.linalg.det(Covar)) + (Xtrain.shape[0] / 2) * np.log(2 * np.pi)
    nmll += (1/2) * (np.matmul(np.matmul(Ytrain_t, Covar_inv), Ytrain)[0][0])
    return nmll
```

Optimize and Train

- Make the initial guess, and use scipy.optimize.minimize to minimize the negative marginal log likelihood I have constructed. Also, I set the constraint for the hyperparameters. All the hyperparameters should be inside (1e-8, 1e8).
- After minimizing, we can get the best hyperparameters for kernel. Then use them to do gaussian process and prediction again.

```
else:

initial_guess = [1.0, 1.0]

result = opt.minimize(fun=NegativeMarginalLogLikelihood, x0=initial_guess, \
bounds = ((1e-8, 1e8), (1e-8, 1e8)), args = (Xtrain, Ytrain, noise_var))

if result.success:

sigma, gamma = result.x[0], result.x[1]

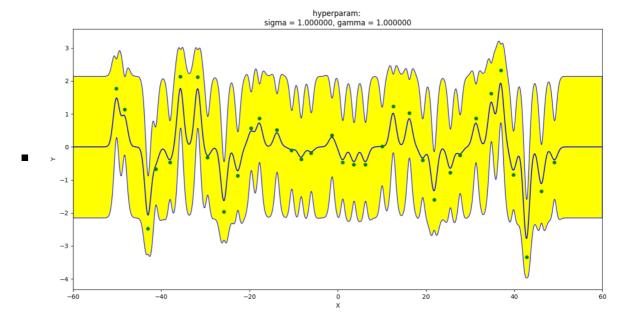
means, variances = prediction(Xtrain, Xtest, Ytrain, noise_var, sigma, gamma)

else:

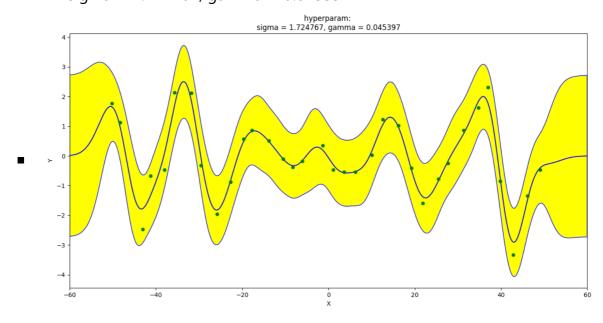
raise ValueError(result.message)
```

b. experiments settings and results

- Part1
 - Set kernel hyperparameter to default value
 - hyperparameter value is:
 - sigma = 1.000000, gamma = 1.000000



- Part2
 - Optimize kernel hyperparameter by minimizing negative marginal loglikelihood
 - hyperparameter value is:
 - sigma = 1.724767, gamma = 0.045397



c. observations and discussion

- For both Part1 and Part2, we can find that if the **training points have appeared in certain x value**, then we will be **more confident of guessing the y value** for that x value. That is, the **variance will be lower** when there are **training point located around**.
- However, if there is **no training data located around**, **the variance will be higher** because we have **less information** to guess the y value for that x value.
- For example, the variance around 0 is small, but the variance around 60 is large.
- For Part1, the hyperparameters for kernel function are **randomly set**, so it will **not fit the training points well**. We can find that the **curve is tortuous**, and the **variance is**

high as long as there is no training points around. Hence, this **model may be underfitting** because the kernel cannot show the correlation between training points well. However, it **gains more flexibility** to guess y value.

• For Part2, the graph is **more smooth** than Part1 because the model can **fit the training points better**. Therefore, the training points are more likely located on the mean curve, and the **variance will be smaller due to the well-defined kernel**. That is, the kernel can display the similarity relation between points well. However, **this model may be overfitting** because it **loses more flexibility** to guess y value.

II. SVM

a. code with detailed explanations

- Part1
 - o Train
 - First, I **construct an SVM problem** by our training features and labels. Then **train an SVM model from SVM problem** by using the SVM parameter.

```
60 ∨ def train(Xtrain, Ytrain, option='', iskernel=False):
         Training a SVM model.
         Args:
             Xtrain: Features of training datas.
             Ytrain: Labels of training datas.
             iskernel: True if the kernel is user-defined.
66
             option: hyperparameters for training.
         Return Value:
70
             A SVM model if not use cross validation.
71
             Accuracy if use cross validation.
         prob = svm_problem(Ytrain, Xtrain, iskernel)
         param = svm parameter(option)
         res = svm_train(prob, param)
76
         return res
```

Predict

■ I use the SVM model which is trained by **train function**. Then **applying the testing features and labels** for the model to get accuracy.

```
def predict(Xtest, Ytest, model):
    """

poing the prediction for testing data.
Args:
    Xtest: Features of testing datas.
    Ytest: Labels of testing datas.
    model: The model which is used to predict.

Return Value:
    p_acc: a tuple including accuracy (for classification), mean-squared error, and squared correlation coefficient (for regression).

"""
return sym predict(Ytest, Xtest, model)[1]
```

Different Kernel functions

- For each kernel function, I use **-s 0** to set the type of SVM to C-SVC (softmargin SVM), **-t** to define which kernel to apply (linear, polynomial, RBF kernel are corresponding to 0, 1, 2, respectively), **-q** to enable quite mode. After setting those options, I can train three kinds of model, and make prediction by applying testing data to the models.
- I use **Accuracy**, **Mean-Squared Error**, and **Time spent** to compare the performance of different kernel functions.

```
if Mode == 1:
    print("-------[Log]: Basic C-SVC for three types of kernel------")
for ktype in range(0,3):
    print("Kernel Type =", kernel_type[ktype])
    print("Kernel Function =", kernel_function[ktype])
    print("SVM type = C-SVC")

start = time.time()

SVMmodel = train(Xtrain, Ytrain, '-s 0 -t {} -q'.format(str(ktype)), False)

PredictRes = predict(Xtest, Ytest, SVMmodel)

stop = time.time()

print("Mean-Squared Error (MSE) =", PredictRes[1])
    print("Time spent = ", stop-start, "s\n", sep="")
```

• Part2

cross validation train

Because I set -v option which will enable cross validation, the return value of train function will be the accuracy of cross validation. Then I compare the cross validation with the current best accuracy to decide whether we should replace the option.

- GridSearch (Not include precomputed kernel)
 - For every kernel, set -v 5 to implement 5-fold cross validation when training.
 - After trying different combination of options, we can figure out which combination makes the best accuracy.

```
def GridSearch(Xtrain, Ytrain, ktype):
112
113
          Use grid search to find the best parameter for training.
114
115
              Xtrain: Features of training datas.
116
              Ytrain: Labels of training datas.
117
              ktype: The type of the kernel.
118
          Return Value:
119
120
              opt_acc: The optimal accuracy in cross validation set.
121
              opt_option: The option for optimal accuracy.
122
123
          k \text{ fold} = 5
          opt_acc = 0
124
125
          opt option = ''
126
          gamma = [ 10 ** power for power in range(-3, 2) ]
127
          coef0 = [ 10 ** power for power in range(-1, 3) ]
128
          cost = [ 10 ** power for power in range(-2, 3) ]
129
          degree = [ deg for deg in range(2, 5) ]
130
          ### grid search start ###
131
132
          print("Kernel Type =", kernel type[ktype])
          print("Kernel Function =", kernel function[ktype])
          print("SVM type = C-SVC")
134
```

• linear kernel: we only need to iterate the cost, which is the importance of the slack in C-SVC.

polynomial kernel: we need to iterate **cost**, **degree of polynomial**, **gamma** (which is used to control the scale of u' * v), and coef0.

■ RBF kernel: we need to iterate **cost**, **gamma** (which is used to control the scale of $||u-v||_2^2$) .

Perform the best hyperparameter

After getting the best hyperparameters of the kernel functions by grid search, I apply these options to train the models and make the prediction.

Part3

o linear kernel

- I construct the linear kernel by the following equation:
 - kernel = u * v'

o RBF kernel

- I construct the RBF kernel by the following equation:
 - $\blacksquare \ kernel = exp(-\gamma*||u-v||_2^2)$

Grid Search (precomputed kernel)

■ Precomputed kernel: we need to iterate cost, gamma because we combine linear kernel with RBF kernel. For every iteration, I compute the kernel with certain gamma, and implement it as training features. Also, I set is_kernel to be true to make sure that we use precomputed kernel when training.

Run linear kernel + RBF kernel

- After precomputing our kernel, I use np.hstack to append the row ID in front of the kernel because the ID for kernel matrix is needed. Then we can use this precomputed kernel as training features and the options obtained from grid search to train the model.
- Also, I set -t to be 4 in order to use the user-defined kernel when training.

```
elif Mode == 3:
   ktype = 4
   print("-----[Log]: Grid Search with 5-fold cross validation---
   print("-----[Log]: Grid Search for {}------".format(kernel_type[ktype]))
   best_acc, best_option = GridSearch(Xtrain, Ytrain, ktype)
                                                               ----".format(kernel_type[ktype]))
   print('Best Cross Validation Accuracy = {}%'.format(best_acc))
   print('Best option = \"{}\"'.format(best_option))
print("Start to use best option to train...")
   gamma, cost = best_option.split()[-2], best_option.split()[-1]
   start = time.time()
   linear_k = linear_kernel(Xtrain, Xtrain)
   RBF_k = RBF_kernel(Xtrain, Xtrain, float(gamma))
   kernel = np.hstack((np.arange(1, 5001).reshape(-1,1), linear_k + RBF_k))
   SVMmodel = train(kernel, Ytrain, '-s 0 -t {} -c {} -g {} -q'.format(str(ktype), str(cost), str(gamma)), True)
   linear test = np.transpose(linear kernel(Xtrain, Xtest))
   RBF_test = np.transpose(RBF_kernel(Xtrain, Xtest, float(gamma)))
   kernel_test = np.hstack((np.arange(1, 2501).reshape(-1,1), linear_test + RBF_test))
   PredictRes = predict(kernel_test, Ytest, SVMmodel)
   stop = time.time()
   print("Mean-Squared Error (MSE) =", PredictRes[1])
   print("Time spent = ", stop-start, "s\n", sep="
```

b. experiments settings and results

• Part1

Use default option and C-SVC mode to train different kernel functions

```
Kernel Type = linear
Kernel Function = u'*v
SVM type = C-SVC
Accuracy = 95.08% (2377/2500) (classification)
Mean-Squared Error (MSE) = 0.1404
Time spent = 3.2166502475738525s
Kernel Type = polynomial
Kernel Function = (gamma*u'*v + coef0)^degree
SVM type = C-SVC
Accuracy = 34.68% (867/2500) (classification)
Mean-Squared Error (MSE) = 2.6212
Time spent = 27.660475969314575s
Kernel Type = radial basis function (RBF)
Kernel Function = exp(-gamma*|u-v|^2)
SVM type = C-SVC
Accuracy = 95.32% (2383/2500) (classification)
Mean-Squared Error (MSE) = 0.1492
Time spent = 6.672668695449829s
```

	linear	polynomial	RBF
Accuracy	95.08%	34.68%	95.32%
MSE	0.1404	2.6212	0.1492
Time Spent	3.2167	27.660	6.6727

• Part2

o Use grid search for finding parameters of the best performing model

- **Cost** is selected from $[10^{-2}, 10^{-1}, 10^{0}, 10^{1}, 10^{2}]$
- **Gamma** is selected from $[10^{-3}, 10^{-2}, 10^{-1}, 10^{0}, 10^{1}]$
- lacktriangle Degree is selected from [2,3,4]
- **Coef0** is selected from $[10^{-1}, 10^0, 10^1, 10^2]$
- Linear Kernel
 - cost = 0.01

Polynomial Kernel

■ cost = 0.01, degree = 3, gamma = 10, coef0 = 100

RBF Kernel

cost = 100, gamma = 0.01

	linear	polynomial	RBF	linear + RBF
Cross Validation Accuracy	97.08%	98.22%	98.26%	97.08%
Test Accuracy	95.96%	97.92%	98.16%	95.64%
MSE	0.1256	0.0568	0.0504	0.118
cost (paramter)	0.01	0.01	100	0.1
gamma (paramter)	-	10	0.01	10
degree (paramter)	-	3	-	-
coef0 (paramter)	_	100	-	-

• Part3

Use linear + RBF kernel

■ cost = 0.1, gamma = 10

■ The table for comparison is together with Part2.

c. observations and discussion

- Part1
 - For default options, polynomial kernel cannot perform well as same as linear kernel and RBF kernel. I think the reason is that polynomial kernel is more

- **complicated** (It has more parameters), if we don't set the parameters properly, it cannot display the similarity relation well for the training data.
- Both linear kernel and RBF kernel has high accuracy even though we use default options.
- Linear kernel is faster than other kernels due to its simple architecture.

• Part2

- Compare to Part1, we can find that polynomial kernel gains a lot of accuracy if
 we find a proper parameters. The accuracy of Linear kernel and RBF kernel are also
 improved. Hence, I believe that the parameters are significant for the SVM
 model. If we can find the proper parameter, these three kernel can all perfrom well.
- Because I implement 5-fold cross validation on training, our svm models are not
 easy to overfit the training datas. Hence, the cross validation accuracy is highly
 related to test accuracy in this experiment.
- The accuracy reduces a little for testing data because the optimal parameters are for training datas, not for testing datas.
- The slack influences a lot for RBF kernel because the cost is high. However, it is not so important for other two kernels.

• Part3

- Although linear+RBF kernel has high accuracy, it doesn't perform better than linear kernel or RBF kernel even though I apply grid search for it in this experiment. Moreover, it takes more time to train than other two kernels.
- Linear+RBF kernel is more complicated, so it may be more likely to overfit. This may lead to the result that it doesn't fit better than linear kernel and RBF kernel.