M4-L2-P2

October 1, 2023

1 Problem 5 (5 points)

Here we will revisit the phase diagram problem from the logistic regression module. Your task will be to code a one-vs-rest support vector classifier.

Work through this notebook, filling in code as requested, to implement the OvR classifier.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap
from sklearn.svm import SVC

x1 = np.array([7.4881350392732475,16.351893663724194,22.427633760716436,29.
 ↪04883182996897,35.03654799338904,44.45894113066656,6.375872112626925,18.
 ↪117730007820796,26.036627605010292,27.434415188257777,38.71725038082664,43.
 ↪28894919752904,7.680445610939323,18.45596638292661,17.110360581978867,24.
 ↪47129299701541,31.002183974403255,46.32619845547938,9.781567509498505,17.
 ↪90012148246819,26.186183422327638,31.59158564216724,35.41479362252932,45.
 ↪805291762864556,3.182744258689332,15.599210213275237,17.833532874090462,33.
 ↪04668917049584,36.018483217500716,42.146619399905234,4.64555612104627,16.
 ↪942336894342166,20.961503322165484,29.284339488686488,30.98789800436355,44.
 ↪17635497075877,])
x2 = np.array([0.11120957227224215,0.1116933996874757,0.14437480785146242,0.
 ↪11818202991034835,0.0859507900573786,0.09370319537993416,0.
 ↪2797631195927265,0.216022547162927,0.27667667154456677,0.27706378696181594,0.
 ↪2310382561073841,0.22289262976548535,0.40154283509241845,0.
 ↪4063710770942623,0.427019677041788,0.41386015134623205,0.46883738380592266,0.
 ↪38020448107480287,0.5508876756094834,0.5461309517884996,0.5953108325465398,0.
 ↪5553291602539782,0.5766310772856306,0.5544425592001603,0.705896958364552,0.
 ↪7010375141164304,0.7556329589465274,0.7038182951348614,0.7096582361680054,0.
 ↪7268725170660963,0.9320993229847936,0.8597101275793062,0.9337944907498804,0.
 ↪8596098407893963,0.9476459465013396,0.8968651201647702,])
X = np.vstack([x1,x2]).T
y = np.
 ↪array([0,2,2,2,2,2,0,2,2,2,2,2,0,0,2,0,1,2,0,0,1,1,1,2,0,1,0,1,1,1,0,0,1,1,1,1,])


def plot_data(X, y, title="Phase of simulated material", newfig=True):
```

```python
    xlim = [0,52.5]
    ylim = [0,1.05]
    markers = [dict(marker="o", color="royalblue"), dict(marker="s",␣
↪color="crimson"), dict(marker="^", color="limegreen")]
    labels = ["Solid", "Liquid", "Vapor"]

    if newfig:
        plt.figure(dpi=150)

    for i in range(1+max(y)):
        plt.scatter(X[y==i,0], X[y==i,1], s=60, **(markers[i]),␣
↪edgecolor="black", linewidths=0.4,label=labels[i])

    plt.title(title)
    plt.legend(loc="upper right")
    plt.xlim(xlim)
    plt.ylim(ylim)
    plt.xlabel("Temperature, K")
    plt.ylabel("Pressure, atm")
    plt.box(True)

def plot_ovr_colors(classifiers, res=40):
    xlim = [0,52.5]
    ylim = [0,1.05]
    xvals = np.linspace(*xlim,res)
    yvals = np.linspace(*ylim,res)
    x,y = np.meshgrid(xvals,yvals)
    XY = np.concatenate((x.reshape(-1,1),y.reshape(-1,1)),axis=1)
    if type(classifiers) == list:
        color = classify_ovr(classifiers,XY).reshape(res,res)
    else:
        color = classifiers(XY).reshape(res,res)
    cmap = ListedColormap(["lightblue","lightcoral","palegreen"])
    plt.pcolor(x, y, color, shading="nearest", zorder=-1,␣
↪cmap=cmap,vmin=0,vmax=2)
    return
```

1.1 Binomial classification function

You are given a function that performs binomial classification by using sklearn's `SVC` tool: `prob = get_ovr_decision_function(X, y, A, kernel, C)`

To use it, input: - `X`, an array in which each row contains (x,y) coordinates of data points - `y`, an array that specifies the class each point in `X` belongs to - `A`, the class of the group (0, 1, or 2 in this problem) – classifies into A or "rest" - `kernel`, the kernel to use for the SVM - `C`, the inverse regularization strength to use for the SVM

The function outputs a decision function (`decision()` in this case), which can be used to evaluate each X, giving positive values for class A, and negative values for [not A].

[ ]:
```python
def get_ovr_decision_function(X, y, A, kernel="linear",C=1000):
    y_new = -1 + 2*(y == A).astype(int)

    model = SVC(kernel=kernel,C=C)
    model.fit(X, y_new)

    def decision(X):
        pred = model.decision_function(X)
        return pred.flatten()

    return decision
```

1.2 Coding an OvR classifier

Now you will create a one-vs-rest classifier to do multinomial classification. This will generate a binomial classifier for each class in the dataset, when compared against the rest of the classes. Then to predict the class of a new point, classify it using each of the binomial classifiers, and select the class whose binomial classifier decision function returns the highest value.

Complete the two functions we have started: - `generate_ovr_decision_functions(X, y)` which returns a list of binary classifier probability functions for all possible classes (0, 1, and 2 in this problem) - `classify_ovr(decisions, X)` which loops through a list of ovr classifiers and gets the decision function evaluation for each point in `X`. Then taking the highest decision function value for each, return the overall class predictions for each point.

[ ]:
```python
def generate_ovr_decision_functions(X, y, kernel="linear", C=1000):
    decisions = []
    classes = np.unique(y)
    for c in classes:
        decisions.append(get_ovr_decision_function(X,y,c,kernel=kernel,C=C))
    return decisions

def classify_ovr(decisions, X):
    results = []
    for decision_fn in decisions:
        results.append(decision_fn(X))

    results = np.array(results)
    maximum = np.max(results, axis=0)
    return np.array([np.where(results[:,i] == maximum[i])[0] for i in␣
 ↪range(len(maximum))]).flatten()
```

1.3 Testing the classifier

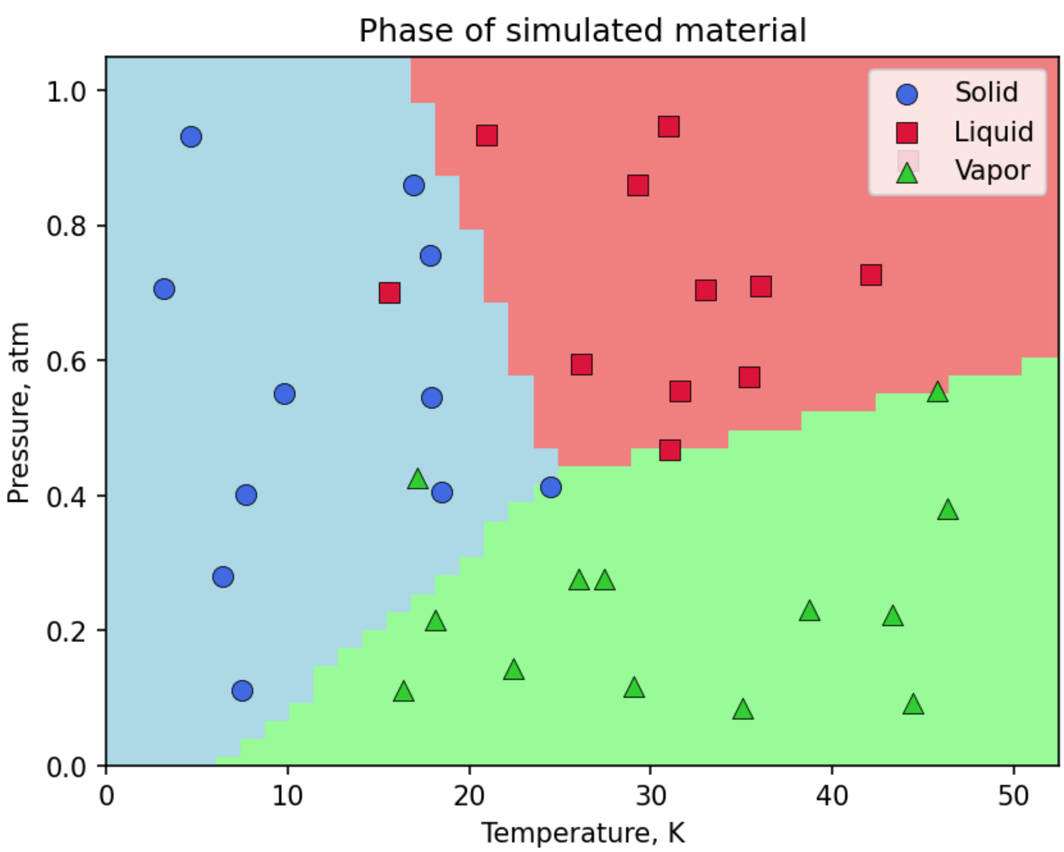
[ ]:
```
kernel = "linear"
C = 1000

decisions = generate_ovr_decision_functions(X, y, kernel, C)
preds = classify_ovr(decisions, X)
accuracy = np.sum(preds == y) / len(y) * 100
print("True Classes:", y)
print(" Predictions:", preds)
print("    Accuracy:", accuracy, r"%")
```

```
True Classes: [0 2 2 2 2 2 0 2 2 2 2 2 0 0 2 0 1 2 0 0 1 1 1 2 0 1 0 1 1 1 0 0 1
1 1 1]
 Predictions: [0 2 2 2 2 2 0 2 2 2 2 2 0 0 0 2 1 2 0 0 1 1 1 2 0 0 0 1 1 1 0 0 1
1 1 1]
    Accuracy: 91.66666666666666 %
```

1.3.1 Plotting results

[ ]:
```
plot_data(X,y)
plot_ovr_colors(decisions)
plt.show()
```



1.4 Modifying the SVC

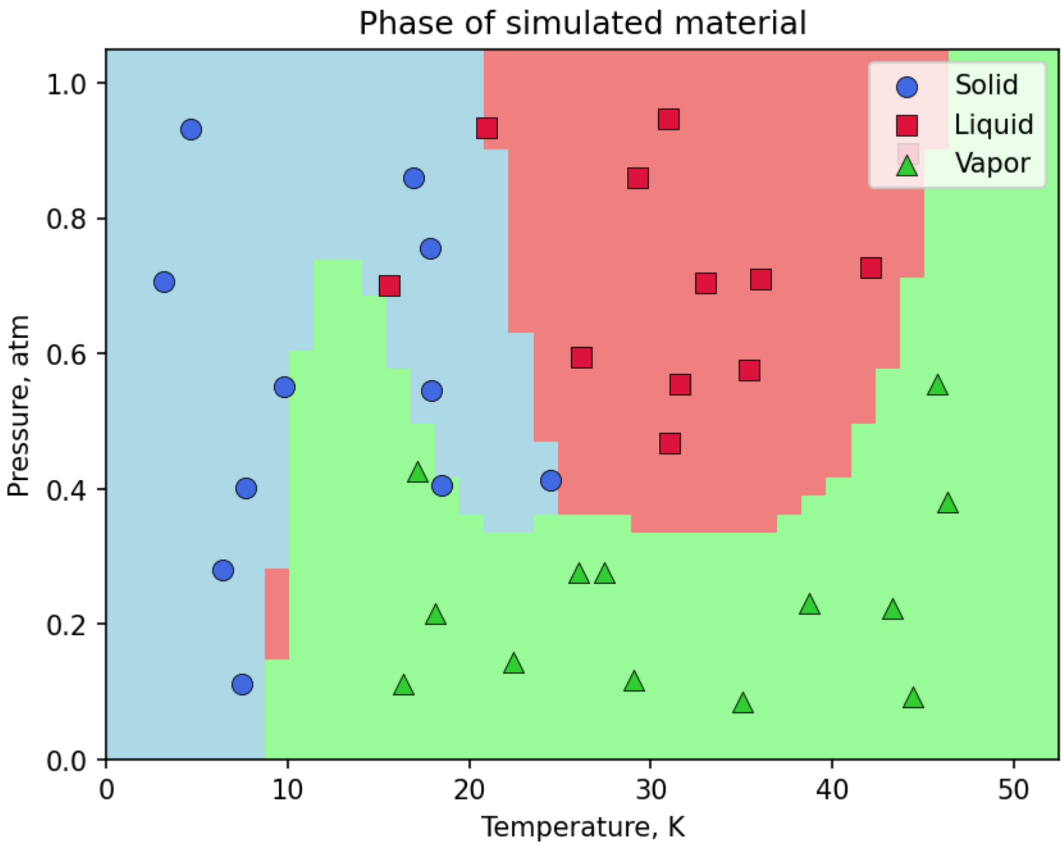
Now go back and change the kernel and C value; observe how the results change.

[ ]:
```
kernel = "rbf"  # CHANGE THIS
C = 100000            # CHANGE THIS

decisions = generate_ovr_decision_functions(X, y, kernel, C)
preds = classify_ovr(decisions, X)
accuracy = np.sum(preds == y) / len(y) * 100
print("True Classes:", y)
print(" Predictions:", preds)
print("    Accuracy:", accuracy, r"%")

plot_data(X,y)
plot_ovr_colors(decisions)
plt.show()
```

```
True Classes: [0 2 2 2 2 2 0 2 2 2 2 2 0 0 2 0 1 2 0 0 1 1 1 2 0 1 0 1 1 1 0 0 1
1 1 1]
 Predictions: [0 2 2 2 2 2 0 2 2 2 2 2 0 2 2 0 1 2 0 0 1 1 1 2 0 0 0 1 1 1 0 0 0
1 1 1]
    Accuracy: 91.66666666666666 %
```


Phase of simulated material
Solid
Liquid
Vapor
Pressure, atm
Temperature, K
1.0
0.8
0.6
0.4
0.2
0.0
0
10
20
30
40
50