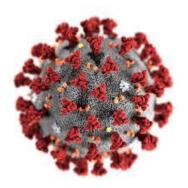
# HW2: Algorithm Implementation and Basic Model Selection Goal

This assignment is the second of three mini projects that will guide you in your task of stopping the spread of disease around the globe!

In this assignment you will implement Soft-SVM using gradient descent. You will also practice basic hyperparameter tuning (model selection) using three algorithms: k-NN, Decision Trees (with ID3), and Soft-SVM.

Many techniques and ideas from this assignment will greatly help you in Major HW3.

#### **Good Luck!**



# **Instructions**

#### Submission

- Submit by: Monday, 06.06.2022, 23:59.
  - Late submissions will be accepted until 07.06.2022 and penalized 5pts.

#### Python environments and more

- We recommend using jupyter notebooks. <u>Google colab</u> can be very convenient since
  it does not require installing anything on your local computer. It will also help you to
  collaborate with your partner online.
- Initial notebook here.
  - Demonstrates how to upload a dataset to Google colab and how to download files from Google colab.
  - You can save a copy of this notebook to your Google drive.
- However, you can use any Python IDE you choose. For working locally with an IDE, we recommend first installing <u>conda</u> for package management (with Python 3.6 or 3.8), and then installing an IDE like <u>PyCharm</u> or <u>Spyder</u>.

#### Your code

- Should be clearly and briefly documented.
- Variables/classes/functions should have meaningful names.
- Will be partially reviewed and graded.

#### Final report

- Should be written in a word processor (Office Word, Google docs, etc.).
  - Should not contain the code itself.
  - Do not submit jupyter notebooks as PDFs.
- Can be in Hebrew, English, or both.
- You are primarily assessed based on your written report.
- Answer the questions in this instruction file according to their numbering.
- Add concise explanations, figures (outputs of your code), tables, etc.
- You are evaluated for your answers but also for clarity, readability, and aesthetics.
- Tables should include feature names and suitable titles.
- Plots should have suitable titles, axis labels, legends, and grid lines (when applicable)
  - We recommend adjusting the default font sizes of matplotlib (see snippet in HW1).

- Submit a zip file containing (please use hyphens, not underscores):
  - The report PDF file with all your answers, named id1-id2.pdf.
    - Do not include your code in your report.
  - Your code:
    - Working with jupyter: a notebook with your code, id1-id2.ipynb.
    - Working with a "traditional" IDE: <u>all</u> relevant python scripts.
    - The following files:
      - SoftSVM.py: your completed SVM module (=class).
      - prepare.py: your <u>updated</u> data preparation pipeline (including normalization).
    - Do not submit csv files.

# **Preliminary: Data Loading**

**Task**: Follow the procedure below.

a. Start by **loading** the <u>preprocessed</u> data from the previous assignment.

**Note:** in Lecture 08 we explain why some preprocess steps (e.g., normalization), should be applied to the validation folds according to statistics computed on the train fold. Here, for simplicity <u>only</u>, you compute these statistics according to the <u>all the training samples</u> (before splitting it to train and validation folds).

b. Make sure the data is **partitioned** correctly to train and test, according to the instructions in the previous assignment.

The train-test partitions **must** be identical to the ones you used in HW1.

- c. Important: do not use the test set in this assignment.
- d. Make sure you did not delete the following features: PCR\_{01, 04, 05, 08, 10}, sport\_activity, and sugar\_levels. Note that there are other important features. Here we chose to specify only some of them. If you deleted some of them, you should edit your preprocessing pipeline accordingly.
- e. Make sure all target variables follow the  $\{+1,-1\}$  convention (rather than  $\{1,0\}$  or  $\{True,False\}$ ).

# Part 1: Basic model selection with k-Nearest Neighbors

Like in the previous HW, we start with the simple k-NN model and use it to practice some new concepts, like model selection. In this part we will use k-NN on PCR\_08 and PCR\_10 to predict the risk, similarly to HW1. You should use sklearn.neighbors.KNeighborsClassifier rather than your custom implementation from the previous HW.

### **Visualization and basic analysis**

Task: Create a temporary DataFrame containing only PCR 08 and PCR 10.

**Reminder:** Use the preprocessed (normalized) <u>training</u> set.

- (Q1) Attach a jointplot of PCR 08, PCR 10 (use the risk class as the hue argument).
- (Q2) Train a k-NN model using k = 1 on your training set and use the updated visualize\_clf method (given in this HW) to visualize the resulted decision regions. Make sure to have appropriate title and labels.

#### **Model selection**

Most ML models are characterized by a set of parameters that control the learning process and are <u>not</u> optimized during training (e.g., k in k-NN and  $max_depth$  in decision trees). As we learned, these hyperparameters can change the learning dynamics dramatically. Hyperparameters are often tuned using <u>k-fold-cross-validation</u>, where we split the training data into  $k_v$  folds and train  $k_v$  models – each trained on  $k_v - 1$  folds and use the last fold for validation (i.e., performance evaluation). This procedure <u>estimates</u> the model's performance on unseen data; thus, we can find the (estimated) optimal hyperparameters.

Note: **DO NOT** use the test set for hyperparameter tuning.

(Q3) Use sklearn.model selection.cross validate to find the best k (neighbours) value in list(range(1, 20, 1)) + list(range(20, 300, 10)) for predicting the risk class using PCR 08 and PCR 10.

If you wish to see clearer trends, you can use higher values than 300, e.g., 500.

Use the (default) accuracy metric and 8-folds to perform cross-validation.

Using the outputs of  $cross\_validate$ , plot a *validation curve*, i.e., the (mean) training and validation accuracies (y-axis) as a function of the k values (x-axis). Add the plot to your report.

**Answer:** which k value is the best? What are its mean training and validation accuracies (computed during the cross validation)? Also explain which k values cause overfitting and underfitting (and why is that).

- (Q4) Use the optimal hyperparameter combination you found and retrain a k-NN model on all the training samples. In your report: plot the decision regions of this final model and write its <u>test</u> accuracy (computed on the separate test split) of this model.
- (Q5) Use the updated visualize\_clf method to visualize the risk decision regions for a k-NN model with k = 1 and one with the best k value from the previous question. Compare these two k-values and discuss the results (2-3 sentences).
- (Q6) Repeat (Q3) but use <u>all</u> the features in your training dataset (instead of only PCR\_08 and PCR\_10). Add the validation curve to your report. Discuss in detail the differences between the results here to those of (Q3) and try to explain them in light of the mechanism of k-NN models.

# Part 2: Decision trees

In this part we will focus on predicting the <u>covid</u> class using decision trees. Rather than implementing the models by yourself, you will use <u>sklearn's DecisionTreeClassifier</u> with entropy as a splitting criterion (ID3) and focus on hyperparameter tuning and visualization.

### Visualization and basic analysis

- (Q7) Return to your report / notebook for HW1. Based on your analysis there (especially in Q28), specify here 4-5 features that seemed important for predicting the covid class. Attach here the plots that made you believe these features are indeed helpful.
- (Q8) Compute the 10 most correlated <u>features</u> to the covid class and attach them to your report.
- (Q9) Train a model with ID3 and max\_depth=4 (not including the root level; use the entire training set, i.e., all the features after preprocessing from all the training samples). What is the training accuracy?
  Visualize the trained tree using plot\_tree (provide feature and class names; use filled=True) and attach the plot to your report. The plot should be readable!
- (Q10) Is the "importance" of the features you named in (Q7) noticeable from the correlation computation in (Q8)?Were these same features used by ID3 in the decision tree built in (Q9)?Compare and discuss your findings (about ½ a page, including appropriate small

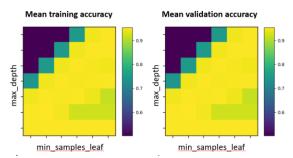
figures).

#### **Model selection**

It is time to search for the best tree to fight covid! Using the <a href="DecisionTreeClassifier">DecisionTreeClassifier</a> documentation, understand how the <a href="min\_samples\_leaf">min\_samples\_leaf</a> argument can mitigate overfitting. You will now tune <a href="two">two</a> hyperparameters <a href="simultaneously">simultaneously</a> — both <a href="min\_samples\_leaf">min\_samples\_leaf</a> and <a href="min\_max\_depth">max\_depth</a>. You need to look for the <a href="combination">combination</a> of these two hyperparameters that lead to the best <a href="walidation">validation</a> performance. There are many approaches for tuning multiple hyperparameters, and here we take the <a href="min\_graph">grid search</a> approach (shortly explained <a href="min\_max\_here">here</a>).

- (Q11) Using 8-fold cross-validation, tune the two aforementioned hyperparameters by performing a grid search (see <a href="GridSearchCV">GridSearchCV</a>). Find the combination yielding the best validation error for predicting the covid class. You should:
  - a. Choose appropriate ranges for both hyperparameters. This may require a few attempts. To make things quicker when trying to find appropriate hyperparameter ranges, you can start by using only 2 folds.
  - b. Since we tune two hyperparameters, instead of a validation curve, plot two heatmaps (<a href="seaborn">seaborn</a> / <a href="pyplot">pyplot</a>), one for the cross-validated training accuracy and one for the cross-validated validation accuracy.

These heatmaps should roughly have the following style / structure:



Make sure to plot the appropriate "ticks" on both axes and use annotations (annot=True) to explicitly write the accuracies inside the heatmap cells.

**Important:** The plots should be readable and informative!

- c. Add the 2 plots to your report and specify which hyperparameter combination is optimal.
- d. Write a hyperparameter-combination that causes underfitting.
- e. Write a hyperparameter-combination that causes <u>overfitting</u>.
- f. Add a <u>short</u> discussion regarding why each specific hyperparameter-combination from sub-questions 'd' and 'e' resulted in under/over-fitting.
- (Q12) Use the optimal hyperparameter combination you found and retrain a decision tree on all the training samples. In your report: plot the decision regions of this final model and write its test accuracy of this model.

# Part 3: Linear SVM and the Polynomial kernel

In this part we will implement a Soft-SVM classifier to better understand this model. We will use gradient-based optimization to find the optimal parameter. Recall that using the whole dataset to perform one step update is costly. To mitigate this problem, we will implement the <u>Stochastic</u> Gradient Descent (SGD) algorithm.

### Implementation of the loss and its gradient

Recall the Soft-SVM formulation:

$$\underset{\boldsymbol{w} \in \mathbb{R}^d, b \in \mathbb{R}}{\operatorname{argmin}} \quad \underbrace{\|\boldsymbol{w}\|_2^2 + C \sum_{i=1}^m \max\{0, 1 - y_i(\boldsymbol{w}^{\mathsf{T}}\boldsymbol{x}_i + b)\}}_{\triangleq p_C(\boldsymbol{w}, b)}$$

Following is the analytic sub-gradient of the objective function above

$$\nabla_{\boldsymbol{w}} p_{\boldsymbol{C}}(\boldsymbol{w}, b) = 2\boldsymbol{w} + C \sum_{i=1}^{m} f(y_{i}(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_{i} + b)) y_{i} \boldsymbol{x}_{i}, \text{ where } f(z) = \begin{cases} -1, & z < 1 \\ 0, & z \ge 1 \end{cases}$$

$$\frac{\partial}{\partial b} p_{\boldsymbol{C}}(\boldsymbol{w}, b) = C \sum_{i=1}^{m} f(y_{i}(\boldsymbol{w}^{\mathsf{T}} \boldsymbol{x}_{i} + b)) y_{i}$$

Task: Copy the SoftSVM module from the given SoftSVM.py into your notebook / project.

<u>Task</u>: Complete the (static) SoftSVM.loss method in the module, so that it computes the objective loss  $p_C(w,b)$  on a given dataset.

Remember: w is a vector and b is a scalar.

**Tip:** When possible, prefer vector operations (e.g., np.sum, np.sign, np.maximum). Avoid using for loops.

<u>Task</u>: Complete the (static) SoftSVM.subgradient method in the module, so that it computes the analytic sub-gradients  $\nabla_w p_{\mathcal{C}}(w,b)$  and  $\frac{\partial}{\partial b} p_{\mathcal{C}}(w,b)$  described above.

**Tip:** When possible, prefer vector operations (e.g., np.sum, np.sign, np.maximum). Avoid using for loops.

### Loading a synthetic dataset for basic experiments

For the few following questions, we will need a toy dataset which is almost linearly separable.

<u>Task</u>: Create and visualize a <u>moon dataset</u> using the following code snippet. For the random state (highlighted), use the same seed as you used in HW1 for splitting the data (created from your IDs).

```
from sklearn.datasets import make_moons
X_moons, y_moons = make_moons(n_samples=1000, shuffle=True, noise=0.05, random_state=TODO)
y_moons = ((2 * y_moons) - 1)[:, None]
print(f"{X_moons.shape}, {y_moons.shape}")

plt.figure(), plt.grid(alpha=0.5), plt.title("Synthetic moon dataset")
_ = sns.scatterplot(x=X_moons[:, 0], y=X_moons[:, 1], hue=y_moons[:, 0])
```

(Q13) Attach the resulted plot to your report.

### Verifying your implementation: Numerical vs. analytical gradients

Recall from your calculus course, the definition of the derivative is:

$$f'(x_0) = \lim_{\delta \to 0} \frac{f(x_0 + \delta) - f(x_0)}{\delta}$$

Thus, we can deduce a method to compute the **numerical** partial derivative w.r.t.  $w_i$  by approximating the limit expression with a <u>finite</u>  $\delta$ :

$$\forall i = 1, ..., d: \ \frac{\partial p_C}{\partial w_i} \approx \frac{p_C(\mathbf{w} + \delta e_i, b) - p_C(\mathbf{w}, b)}{\delta} \triangleq u_i, \ \text{ where } e_i = [0, ..., 0, \underbrace{1}_{i-th}, 0, ..., 0]$$

Denote the **numerical** sub-gradient by  $\mathbf{u}_{\delta}(\mathbf{w},b) = \begin{bmatrix} u_1 \\ \vdots \\ u_d \end{bmatrix}$ .

Using the numerical sub-gradient, we will now verify the correctness of your implementation for the loss and its analytic sub-gradient.

We will plot the residuals  $\|\underbrace{\nabla_w p_{\mathcal{C}}(\mathbf{w}, b)}_{\text{analytic}} - \underbrace{\mathbf{u}_{\delta}(\mathbf{w}, b)}_{\text{numeric}}\|_2$  over many repeats as a function of  $\delta$ .

<u>Task</u>: Copy the functions from the given  $verify\_gradients.py$  into your notebook / project. Read and understand these functions <u>but do not edit them</u>.

**(Q14)** Using the synthetic moon dataset, generate a plot that compares the numerical gradients to the analytic gradients. Do this by running the following command:

```
compare_gradients(X_moons, y_moons, deltas=np.logspace(-9, -1, 12))
```

**Important:** Make sure y\_moons follows the {+1, -1} convention.

Attach the plot to your report. Briefly discuss and justify the demonstrated behavior.

### Solving Soft SVM problems using Stochastic Gradient Descent (SGD)

<u>Task</u>: Complete the given SoftSVM.predict method according to the decision rule of linear classifiers (return the predicted labels using the {+1,-1} convention).

**Tip:** prefer vector operations (e.g., np.dot and np.sign) when possible. Avoid using for loops.

Task: Read and understand the given SoftSVM.fit with logs method.

Complete the code inside the loop to perform a gradient step (compute  $g_w$  and  $g_b$  and use them to update w and b).

SGD is an iterative learning algorithm. A common method to analyze such algorithms is to plot a *learning curve*, i.e., plot the accuracy and/or loss of the model over time (i.e., steps).

(Q15) The following snippet trains a SoftSVM model on the synthetic moon dataset and plots the learning curves. Make sure your model <u>converges</u>. For that, you may need to adjust the 1r and max\_iter values. However, you may <u>not</u> change the given c value. Add suitable labels and titles. Finally, add the plot(s) to your report. Also attach a plot of the decision regions of your model (at the end of training).

**Answer:** What is the maximal training accuracy and the minimal training loss achieved by your model? Are they attained at the same step? If so – why? If not – how is it possible?

```
clf = SoftSVM(C=1, lr=2e-4)
losses, accuracies = clf.fit_with_logs(X_moons, y_moons, max_iter=3000)
plt.figure(figsize=(13, 6))
plt.subplot(121), plt.grid(alpha=0.5), plt.title ("TODO")
plt.semilogy(losses), plt.xlabel("TODO"), plt.ylabel("TODO")
plt.subplot(122), plt.grid(alpha=0.5), plt.title ("TODO")
plt.plot(accuracies), plt.xlabel("TODO"), plt.ylabel("TODO")
plt.tight_layout()
```

<u>Submit</u>: Copy your <u>completed</u> SoftSVM module into a separate file called *SoftSVM.py*.

Submit this file at the end of your work.

### Using a feature mapping

We now want to understand the polynomial feature mapping and its corresponding kernel. To make our following explanation clearer, assume we want to use a 2<sup>nd</sup>-degree polynomial feature mapping on a 2-dimensional data (i.e., having two raw features).

#### Recap: solving SVMs with feature mappings

We have two ways to use this feature mapping (we present Hard-SVM for simplicity):

1. Explicitly apply the feature mapping  $\phi(x) = \left[1, \sqrt{2}x_1, \sqrt{2}x_2, \sqrt{2}x_1x_2, x_1^2, x_2^2\right]$  and solve the <u>primal</u> problem in the new 6-dimensional space:

$$\underset{\boldsymbol{w} \in \mathbb{R}^6}{\operatorname{argmin}} \|\boldsymbol{w}\|_2^2 \text{ s.t. } y_i \cdot \boldsymbol{w}^{\mathsf{T}} \boldsymbol{\phi}(\boldsymbol{x}_i) \ge 1, \ \forall i \in [m]$$

2. Use an appropriate kernel function, i.e.,  $K(u,v) = \phi(u)^{T}\phi(v) = (u^{T}v+1)^{2}$ , and solve the <u>dual</u> problem in an m-dimensional space (without explicitly computing the feature mappings):

$$\max_{\alpha \in \mathbb{R}_{+}^{m}} \sum_{i=1}^{m} \alpha_{i} - \frac{1}{2} \sum_{i,j=1}^{m} y_{i} y_{j} \alpha_{i} \alpha_{j} \underbrace{\phi(x_{i})^{\mathsf{T}} \phi(x_{j})}_{=K(x_{i}, x_{j})}$$

We will now use the polynomial feature mapping to predict to predict the <a href="mapping">spread</a> variable using the two features we found on HW1: PCR 05 and sugar levels.

Since you only implemented the <u>primal</u> (Soft-)SVM problem, we will use the **first** way and explicitly transform the aforementioned 2 features into 6 polynomial features.

<u>Task</u>: Use your training set to create a temporary DataFrame containing only PCR\_05, sugar\_levels, and spread.

(Q16) Plot a jointplot of PCR\_05 and sugar\_levels, using spread as the hue.

We now wish to create a <u>single</u> model that: (1) transforms the 2 features into 6 polynomial features and then (2) trains your custom SoftSVM module on these 6 features. To do so, we will use a Pipeline.

The following code snippet creates such a pipeline:

<u>Task</u>: Complete the first step in the pipeline above to make it apply a 2<sup>nd</sup>-degree PolynomialFeatures transformation.

- (Q17) Train such a model 5 times (on all the training samples), using the hyperparameters written in the snippet above. Set the max\_iter to 10,000. Since you work with a pipeline, use the following command to specify a hyperparameter of an inner model inside a pipeline: svm\_clf.fit(X\_train, y\_train, SVM\_max\_iter=10000). In your report:
  - (a) Write the 5 resulting train accuracies, their mean, and their standard deviation.
  - (b) Plot the 5 resulting decision regions (use visualize clf on the training set).
  - (c) Answer: what is (are) the source(s) of the variability in the resulting models (refer also to the convexity of this problem)?
- (Q18) Use 10-folds cross-validation to tune the c hyperparameter. You should choose suitable hyperparameter ranges (tip: use np.logspace) on your own. Keep the lr, max\_iter, and batch\_size fixed as they are in the snippet above. In your report:
  - (a) Specify the range you chose for the tuning process.
  - (b) Attach a suitable *validation curve* to your report (plot both train and validation accuracies). The x-axis should appear in a logarithmic scale. Fully discuss and explain the behavior demonstrated in the plot.
  - (c) Specify the optimal c value and its corresponding (cross validated) train and validation accuracies.
- (Q19) Train your model on all the training samples using the optimal c value you found. In your report: plot the decision regions of this final model and write its test accuracy.

# Part 4: The RBF kernel

#### Before we start: what is the Radial Basis Function kernel?

In Lectures 04 and 05 we presented the RBF kernel (also called the Gaussian kernel). This kernel is often defined as  $K(\boldsymbol{u},\boldsymbol{v}) = \exp\left\{-\frac{1}{2\sigma^2}\|\boldsymbol{u}-\boldsymbol{v}\|_2^2\right\}$  or  $\exp\{-\gamma\|\boldsymbol{u}-\boldsymbol{v}\|_2^2\}$ , which can be decomposed using an <u>infinite</u>-dimensional feature mapping (see the lecture).

Note: If you wish, you can already practice this mapping by solving Q4 in Exam A from the previous semester.

After solving the appropriate  $\underline{2}$  optimization problem, we get a dual solution  $\alpha \in \mathbb{R}^m_+$ . Like we saw in the lecture, given a new datapoint  $x \in \mathbb{R}^d$  for prediction, the model predicts  $h(x) = \operatorname{sign}(\sum_{i=1}^m \alpha_i y_i K(x, x_i)) = \operatorname{sign}(\sum_{i \in [m], \alpha_i > 0} \alpha_i y_i K(x, x_i))$ .

This rule acts similarly to a weighted nearest-neighbor algorithm (on the training set), where "neighborhoods" of datapoints are computed using the kernel function.

For instance, consider a 1-dimensional training dataset:  $\{\underbrace{(0,-1)}_{(x_1,y_1)},\underbrace{(2,+1)}_{(x_2,y_2)},\underbrace{(-1,+1)}_{(x_2,y_2)}\}.$ 

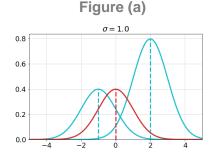
Assume the dual SVM solution is  $\alpha = (1, 1, 2)$ .

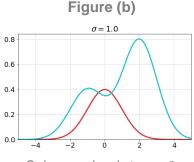
When  $\sigma = 1$ , we get the (weighted) Gaussians on Figure (a).

Given a new datapoint x = 0.5, the model predicts:

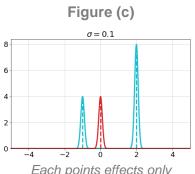
$$\begin{split} h(\mathbf{x}) &= \operatorname{sign} \sum_{i} \alpha_{i} y_{i} K(\mathbf{x}, \mathbf{x}_{i}) = \operatorname{sign} \left( 1 \cdot (-1) \cdot K(0.5, 0) + 1 \cdot 1 \cdot K(0.5, 2) + 2 \cdot 1 \cdot K(0.5, -1) \right) \\ &= \operatorname{sign} \left( -\exp \left\{ -\frac{\|0.5 - 0\|_{2}^{2}}{2} \right\} + \exp \left\{ -\frac{\|0.5 - 2\|_{2}^{2}}{2} \right\} + 2 \exp \left\{ -\frac{\|0.5 - (-1)\|_{2}^{2}}{2} \right\} \right) \\ &= \operatorname{sign} \left( -\exp \left\{ -\frac{0.25}{2} \right\} + \exp \left\{ -\frac{2.25}{2} \right\} + 2 \exp \left\{ -\frac{2.25}{2} \right\} \right) \approx \operatorname{sign} (-0.88 + 0.32 + 0.65) = +1 \end{split}$$

In fact, we can create an even clearer visualization by drawing the weighted <u>sum</u> of positive points' Gaussians (blue) and the one of negative ones (red). See Figure (b). Finally, Figure (c) shows the case resulted Gaussians when  $\sigma = \frac{1}{10}$ . Notice how each training point influences only a small environment around it. We explain this below.





Only very closely to x = 0, the model predicts y = -1.



Each points effects only a small environment around it

As another example, consider a (finite) solution vector  $\alpha \in \mathbb{R}^m_+$  in the extreme case where  $\sigma^2 \to 0$  and  $\gamma \to \infty$ , it can be easily shown that we <u>should</u> get a <u>similar</u> behavior (perhaps up to edge cases) to the <u>1</u>-nearest-neighbor algorithm on the support vectors, i.e., the vectors with corresponding nonzero  $\alpha$  weights:

$$\begin{split} h(x) &= \operatorname{sign}\left(\sum\nolimits_{i \in [m], \alpha_i > 0} \alpha_i y_i K(x, x_i)\right) = \lim_{\gamma \to \infty} \operatorname{sign}\left(\sum\nolimits_{i \in [m], \alpha_i > 0} \alpha_i y_i \exp\{-\gamma \|x - x_i\|_2^2\}\right) \\ &= y_{i^*} \text{ where } i^* = \operatorname{argmin}_{i \in [m], \alpha_i > 0} \|x - x_i\|_2^2 \end{split}$$

To complete our explanations, read this <u>blogpost</u> and then watch this short <u>video</u>. While doing this, keep in mind the prediction rule  $h(x) = \text{sign}(\sum_{i \in [m], \alpha_i > 0} \alpha_i y_i K(x, x_i))$ .

Like we did in Part 1, we now wish to predict the <u>risk</u> variable using PCR\_08 and <u>PCR\_10</u>. This time, we shall use a Kernel SVM with an <u>RBF</u> kernel. Since the corresponding feature mapping is of an <u>infinite</u> dimensionality, we will have to use the kernel trick and solve the <u>dual</u> problem, like we explained <u>2</u>. Our custom SoftSVM class is not suitable for solving the dual formulation, hence we will use <u>sklearn's</u> implementation.

**Task:** Use sklearn.svm.SVC to train an SVM with an RBF kernel on the two features and the <u>risk</u> variable. We first wish to visualize the regularizing effect of  $\gamma$ , so you should begin by fixing c=1e4 and train 10 different models (on the entire training set, i.e., all training samples, narrowed down to the two features) with all  $\gamma$  values in np.logspace (-5, 4, 10).

(Q20) Use our visualization method to visualize the ten models' decision regions (use the marker\_size argument to adjust the plots for small decision regions).

Attach the ten plots to your report (resize them to fit in a single page of your report). Remember that all plots should have suitable titles.

We recommend that you try to understand the exhibited behaviors in these ten plots in light of the explanations at the beginning of this part. You are <u>not</u> required to explain these behaviors in your report.

(Q21) Compare the decision regions of the k-NN model with k = 1 from (Q2) to those of the RBF model with  $\gamma = 10^4$  from (Q20). We expected the two models to be very similar, but we still see significant differences. Try to <u>explain</u> the differences (try to give several reasons, there isn't a single correct answer).

(Q22) Now, given the problem at hand (i.e., predicting the risk using an SVM with the RBF kernel on PCR\_08 and PCR\_10), we wish to find an optimal combination of C and γ. To this end, repeat the grid search steps from (Q11) and perform 8-fold cross validation on C and γ. Remember: to save time, you can use only 2 folds when looking for appropriate ranges for these hyperparameters.
Don't forget to attach here the required plots and explanations, as in (Q11).

(Q23) Use the optimal hyperparameter combination you found and retrain an RBF model on the all the training samples. In your report: plot the decision regions of this final model and write its <u>test</u> accuracy. Compare these results to those from (Q4).

Based on the test accuracy, which model is better for the task of predicting the risk?

# **Submitting the files**

Return to the instructions on Pages 2-3 and make sure you submit <u>all</u> required files.