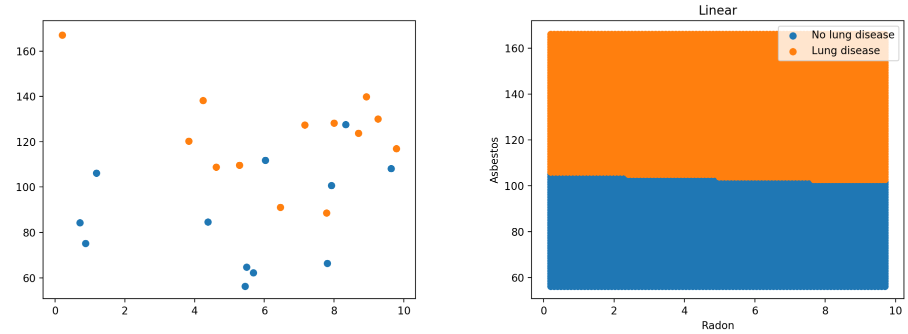
Homework 5 – Machine Learning (CS4342, Whitehill, Spring 2021)

1. **Support Vector Machines (Kernels): [50 points]**: The purpose of this problem is to clarify what it means to train and apply a SVM with a non-linear kernel. To get started, first download the toy dataset `lung_toy.npy` under the Files section on Canvas. In this dataset, there are two features per example (radon, in picoCuries; and asbestos, in kilograms), representing how much of these toxins a person has ingested during their lifetime. The labels (each $y \in \{-1, +1\}$) represent whether or not the person will acquire lung disease as a result of their exposure to radon and asbestos. On all of the problems below, you should use sklearn's `sklearn.svm.SVC` class, which implements a *soft-margin* SVM. To specify how "soft" it is (i.e., how much slack is allowed to the training examples), use the C variable that was defined in the lecture notes.

   All of the exercises below require some scatter-plots; please make sure to give each plot its own title (using `plt.title`) so that it's clear which plot belongs to which exercise. When computing the SVM's predictions over a dense grid of points (I recommend a 100x100 grid of points that evenly covers the range of radon and asbestos values), it is acceptable on this assignment just to use two nested for-loops to iterate over all the points in the grid. (If you wish, it's more efficient to vectorize this using the `np.meshgrid` function; however, this is optional.)

   (a) Using sklearn's `sklearn.svm.SVC` class, train a *linear* SVM on this dataset (set $C = 0.01$). Note that you must explicitly set the `kernel` parameter to `linear` (since the RBF kernel is the default). Even though the data are not linearly separable, since the SVM has a soft margin, the training can still converge. Plot (include it in your PDF) the trained machine's predictions on a 2-D grid of combinations of (radon, asbestos) values, where the color of each point in the scatter-plot indicates the predicted class label. On a *subset* of the training data, the scatter plot of the raw data, and the plot of predictions, would look something like the following:



   Note that the linear SVM does not do a great job of separating the positive from the negative examples.

   (b) In order to potentially fit the data more accurately, try *transforming* each input $\mathbf{x}$ using a non-linear transformation ϕ into a higher-dimensional feature space. In class, I showed several examples of such transformations; see slide #28 from `Lecture16.pdf`, which shows an example for degree-2 polynomial transformations. In this exercise, you should instead define ϕ so that it computes degree-3 polynomial features of $\mathbf{x} = [r \ a]^\top$. More specifically, define ϕ such that $\phi(\mathbf{x})^\top \phi(\mathbf{x}') = (1 + \mathbf{x}^\top \mathbf{x}')^3$ for all $\mathbf{x}, \mathbf{x}'$. You may find a symbolic calculator such as `wolframalpha.com` to be useful (though it's not required). Write down the mathematical expression of your transformation in your PDF. (Hint: it should map from $\mathbb{R}^2$ to $\mathbb{R}^{10}$.) Then apply this transformation to every example in the training set. Next, train an SVM (set $C = 0.01$) on the transformed examples. (Since you are performing the transformation yourself, you should specify the `linear` kernel.) Finally, plot (include it in your PDF) the trained machine's predictions on the same 2-D grid of combinations of the raw (radon, asbestos) values as you did for part (a) above. You should see that the decision boundary between classes – in terms of the *raw* feature space – is now curved. Note that – like always – the SVM training procedure still identifies the hyperplane (a linear separator) with maximum margin; however, this hyperplane now lives in a 10-dimensional space.

(c) Since the SVM optimization function depends only on how the training examples occur within *inner products*, we can thus train the exact same SVM as part (b) both more compactly (less memory) and more quickly (less time) using the "kernel trick": Instead of explicitly transforming each example $\mathbf{x}$ through ϕ, we rather *implicitly* transform *pairs* of training data through a kernel function $k_{\text{poly3}}(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\top \mathbf{x}')^3$. To do so, we need to give the SVM training algorithm (set $C = 0.01$) a matrix consisting of the kernel values for all pairs of training data. Specifically, you should construct a kernel matrix $\mathbf{K}^{\text{tr}} \in \mathbb{R}^{n \times n}$, where n is the number of training examples, such that entry $\mathbf{K}^{\text{tr}}_{ij} = k_{\text{poly3}}(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$. For this exercise, you should **not** use ϕ; rather use k_{poly3} as defined above. Since, in this exercise, you are constructing the kernel matrix yourself, you should initialize an SVM using the `precomputed` kernel type, and pass the kernel matrix $\mathbf{K}^{\text{tr}}$ (instead of the design matrix $\mathbf{X}$) to the `fit` function. Training this SVM with the kernel matrix should result in the *exact same* SVM as for part (b).

Recall that, for non-linear SVMs, the decision function is given by $g(\mathbf{x}) = \sum_{i=1}^{n} \alpha^{(i)} y^{(i)} k(\mathbf{x}, \mathbf{x}^{(i)}) + b$. In other words, the model needs to compute the kernel values between the test example $\mathbf{x}$ and training examples $\mathbf{x}^{(i)}$. Hence, for making predictions using the trained model, you will need to feed the `predict` function another kernel matrix $\mathbf{K}^{\text{te}} \in \mathbb{R}^{n' \times n}$, where n' is the number of examples in the testing set, that contains the kernel values for all possible ordered pairs of examples where the first is from the testing set and the second is from the training set. This reflects the *disadvantage* of using kernels – you must store training examples (though not necessarily all of them, as noted in part (d)) in order to make predictions at test-time. Using this procedure, create another prediction plot (include it in your PDF); it should look identical to part (b).

Note: when computing the kernel matrices above, it is acceptable on this assignment just to use two nested for-loops to compute all kernel values. However, it's more efficient to vectorize this by using numpy's broadcasting capabilities.

(d) Instead of computing the kernel matrix yourself, invoke sklearn's built-in kernel functionality simply by passing `poly` as the `kernel` value to the SVM constructor (set $C = 0.01$). In order to match exactly the ϕ from parts (b) and (c), you should set the `gamma=1`, `coef0=1`, and `degree=3`. Since sklearn is performing the kernel trick for you, you should directly pass the design matrix $\mathbf{X}$ to the `fit` function. Similarly, for prediction, you can also pass just the design matrix containing the raw test examples. The computation of the kernel function is handled by sklearn internally. Better still, the SVM you trained will store *only* the support vectors (those training vectors whose associated Lagrange multipler $\alpha > 0$), which can save a lot of time and memory compared to storing the entire training set. After training your SVM, create another prediction plot (include it in your PDF); it should look identical to parts (b) and (c).

(e) Finally, experiment with the most popular SVM kernel: the Gaussian radial basis function (RBF). Use sklearn's built-in RBF kernel function to train the model (for this part *only*, set $C = 1.0$), and then plot the predictions (include the two plots in your PDF) for $\gamma = 0.1$ and $\gamma = 0.03$. Describe in your PDF how (in qualitative terms) the prediction boundaries differ for the different values for bandwidth hyperparmeter γ; say which one you think is more likely to overfit. **Extra credit (4 points)**: Implement the RBF-SVM yourself (i.e., initialize the SVM using `precomputed` as the kernel type) by creating your own kernel function k_{RBF}. To get the extra credit, you must vectorize the computation of the $\mathbf{K}^{\text{tr}}$ and $\mathbf{K}^{\text{te}}$. Probably the easiest way is to construct two different 3-D arrays of training/testing vectors that are replicated many times and then subtract the arrays; the `np.repeat` and `np.swapaxes` methods are handy.

Put your Python code in a file, called `homework5_WPIUSERNAME.py`, and your PDF file, called `homework5_WPIUSERNAME.pdf` into a Zip file (`homework5_WPIUSERNAME.zip`) and submit it on Canvas.