**Final Report**

Prepared by

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Course: Introduction to Machine Learning

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**Alzheimer's Disease (AD) diagnosis using high-dimensional glucose metabolism measures**

We revisit the problem of Alzheimer's Disease (AD) or the dementia of Alzheimer's type (DAT) diagnosis based on brain glucose metabolism changes. However, instead of just focusing on the glucose metabolism activity in the two particular brain regions, we now consider glucose metabolism measurements taken across several regions of the cerebral cortex of the brain. The cerebral cortex is the outermost layer of the brain and it consists of around 14−16 billion neurons making up approximately 40% of the mass of the brain. The cerebral cortex is divided into two hemispheres and its surface is highly folded. The "peaks" of the folds are called gyri and the "grooves" of the folds are called sulci. Figure 1 illustrates the various regions within the cerebral cortex of a human brain also referred to as "cortical" brain regions.

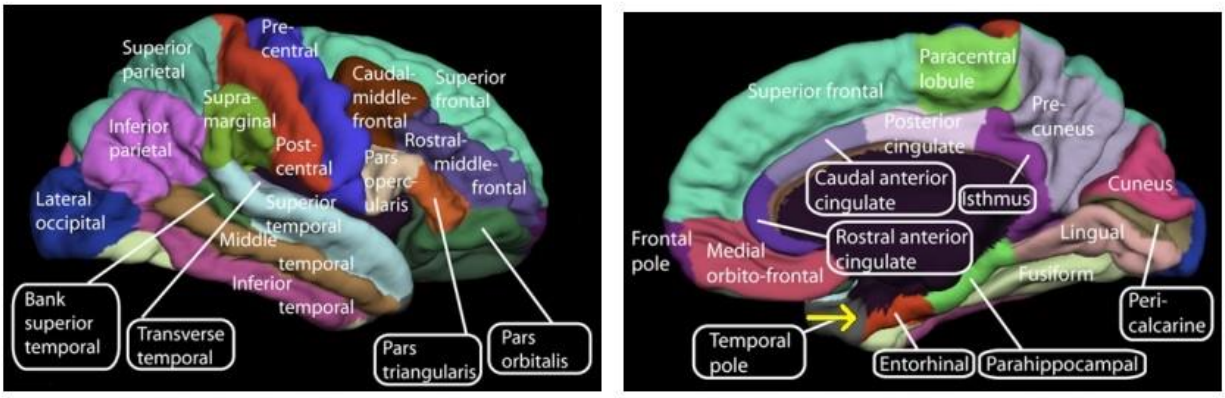



Figure1: Anatomical regions of the cerebral cortex of the human brain. ©Hagmann P, Cammoun L, Gigandet X, Meuli R, Honey CJ, et al. (2008) Mapping the Structural Core of Human Cerebral Cortex. PLOS Biology 6(7): e159.

The specific goal of this project is to develop a support vector machine (SVM) classifier that can predict if an individual belongs to the stable normal controls (sNC) group or the stable DAT (sDAT) group based on a high-dimensional glucose metabolism signature taken from several regions in the individual's brain.

**Data**

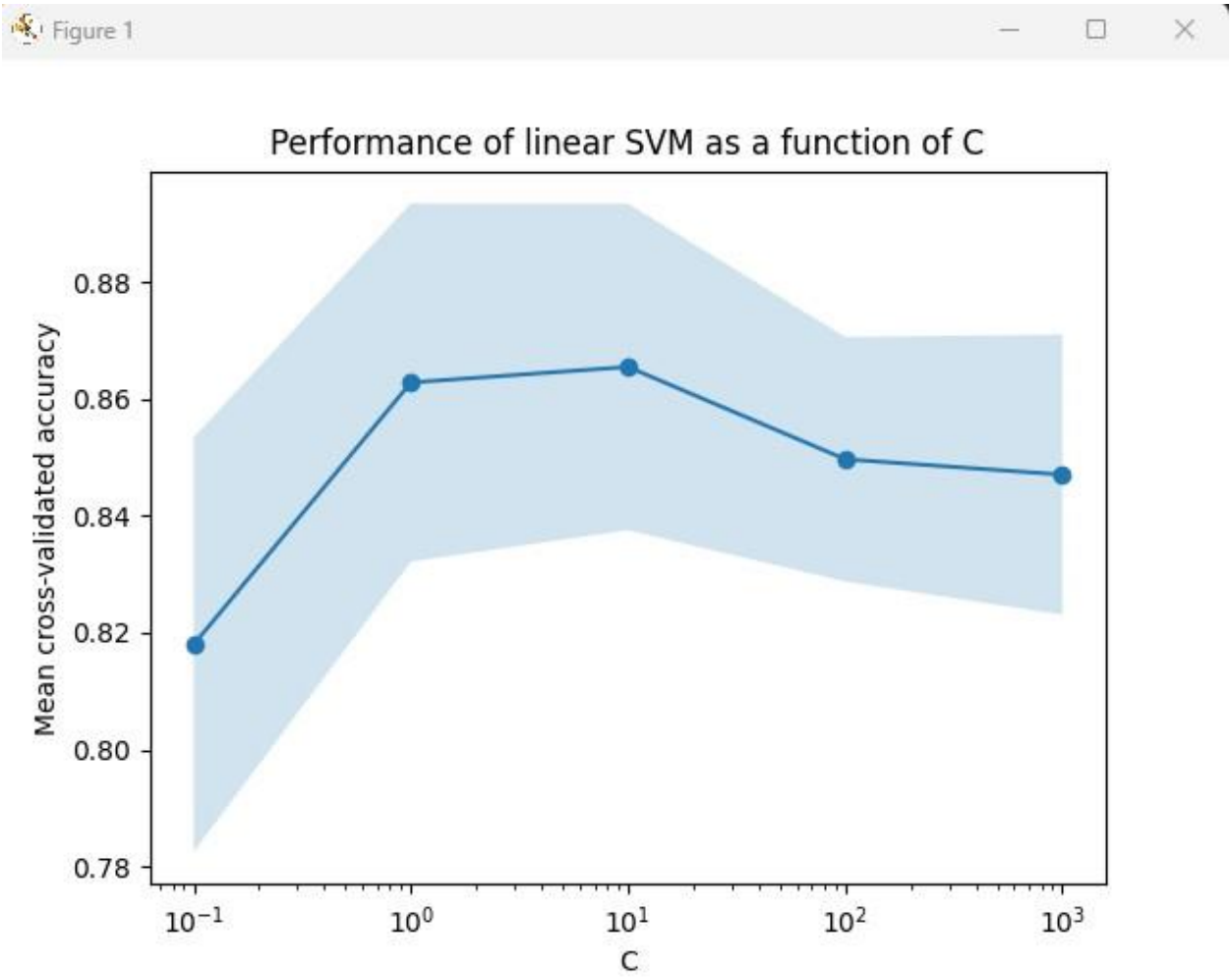
The "training" dataset consists of glucose metabolism features taken from 14 cortical brain regions (see fdg pet.feature.info.txt for a list of these regions) across
237 sNC and 237 sDAT individuals given in *train.fdg_pet.sNC.csv* and *train.fdg_pet.sDAT.csv* respectively. The *test.fdg_pet.sNC.csv* and *test.fdg_pet.sDAT.csv* files correspond to a "test" dataset with the same brain glucose metabolism features taken from another 415 sNC and 122 sDAT individuals respectively.

**Performance reporting convention**

We are reporting accuracy, sensitivity, specificity, precision, recall and balanced accuracy performance metrics when summarizing the performance ("Err") of a classification model.

## Experiment 1: -

First, we train a linear SVM classification model to discriminate between the sNC and sDAT individuals based on the brain glucose metabolism features. We use the "training" dataset and a cross-validation (CV) based grid-search approach to tune the regularization parameter "C" of the linear SVM model. Using the "best" "C" setting, we re-train on the entire "training" dataset to obtain the final linear SVM classification model.




**Performance metrics:**

Best hyperparameter setting: {'C': 10}

Accuracy: 0.8547486033519553

Sensitivity: 0.9426229508196722

Specificity: 0.8289156626506025

Precision: 0.6182795698924731

Recall: 0.9426229508196722

Balanced Accuracy: 0.8857693067351373 Confusion

matrix:

[[344 71]

[ 7 115]]

Classification report:

| | precision | recall | f1-score | support |
|---|---|---|---|---|
| 0.0 | 0.98 | 0.83 | 0.90 | 415 |
| 1.0 | 0.62 | 0.94 | 0.75 | 122 |
| accuracy | | | 0.85 | 537 |
| macro avg | 0.80 | 0.89 | 0.82 | 537 |
| weighted avg | 0.90 | 0.85 | 0.86 | 537 |

**Discussion:**

Plotting the regularisation parameter "C" as a function of the linear SVM classifier's performance. The y-axis displays the mean cross-validated accuracy of the relevant model, while the x-axis displays the values of C utilised in the hyperparameter tuning phase. The standard deviation of the accuracy scores throughout the five folds of the cross-validation is shown by the dark region surrounding the mean accuracy curve.

The graphic shows that, up until a certain point (about C=10), the mean cross-validated accuracy rises as C grows. Following that, accuracy begins to decline when C is raised more. Since bigger values of C have narrower margins and might lead to overfitting to the training data, this behaviour is predicted. Therefore, the maximum accuracy score obtained during the hyperparameter tuning phase, which in this case is C=10, is used to pick the ideal value of C that balances model complexity and accuracy.

## Experiment 2: -

Now, we train a non-linear SVM classifier with a polynomial kernel for the sNC vs sDAT classification task. We use the “training” dataset and a CV based grid-search approach to tune both the regularization parameter “C” as well as the degree “d” parameter of the polynomial kernel. Using the “best” “(C, d)” setting, we re-train on the entire “training” dataset to obtain the final polynomial kernel SVM model.

Performance metrics when using Polynomial kernel SVM:

Accuracy: 0.87

Sensitivity: 0.95

Specificity: 0.85

Precision: 0.65Recall: 0.95

Balanced Accuracy: 0.90

Starting with the polynomial kernel SVM model, it was able to accurately classify 87% of the samples with an accuracy of 0.87 on the test dataset. Additionally, it had a sensitivity of 0.95, which meant that 95% of the people with stable DAT were accurately recognised. In contrast, the model's specificity was 0.85, meaning it accurately recognised 85% of the people with stable normal controls. The model's accuracy was 0.65, which indicates that it correctly identified individuals as belonging to the sDAT group 65% of the time. Recall, sometimes referred to as the true positive rate, was 0.95, meaning that 95% of the people with sDAT were properly identified by the model. The model's balanced accuracy, which accounts for the imbalance between the two classes and provides a more realistic view of its performance, was 0.90 at the end.

The accuracy of the linear SVM model, which was marginally inferior to that of the polynomial kernel SVM model on the test dataset, was 0.85. The model's sensitivity, which was greater at 0.94 and showed that it accurately identified 94% of those with sDAT, was higher. The model's specificity, 0.83, was a little bit lower than that of the polynomial kernel SVM model. The model's accuracy was 0.62, which was less than the polynomial kernel SVM model's. The model's recall and sensitivity both stood at 0.94. Finally, the model's balanced accuracy was 0.89, somewhat less accurate than the polynomial kernel SVM model.

In conclusion, the polynomial kernel SVM model outperformed the linear SVM model in terms of accuracy and balance, but lagged behind in terms of precision and somewhat lagged behind in terms of specificity. It's crucial to remember that the exact objectives and limitations of the

project will ultimately determine which model is used, and that further hyperparameter tuning or testing out several models may result in even greater performance.

## Experiment 3: -

We repeat the above experiment by replacing the polynomial kernel with a radial basis function (RBF) kernel. To note: here the RBF kernel parameter “γ” needs to be tuned instead of the “d” parameter of the polynomial kernel.

Performance metrics when using RBF kernel SVM:

Accuracy: 0.8734

Sensitivity: 0.9426

Specificity: 0.8530

Precision: 0.6534

Recall: 0.9426

Balanced Accuracy: 0.8978

Performance metrics when using Polynomial kernel SVM:

Accuracy: 0.87

Sensitivity: 0.95

Specificity: 0.85

Precision: 0.65Recall: 0.95

Balanced Accuracy: 0.90

Performance metrics when using Linear kernel SVM:

Accuracy: 0.8547486033519553

Sensitivity: 0.9426229508196722

Specificity: 0.8289156626506025

Precision: 0.6182795698924731

Recall: 0.9426229508196722

Balanced Accuracy: 0.8857693067351373

The accuracy of the RBF kernel SVM model is 0.8734, which is more than the accuracy of the linear SVM model (0.8547) and the polynomial kernel SVM model (0.87). In addition, the RBF kernel SVM outperforms the other two models in terms of balanced accuracy (0.8978) and sensitivity (0.9426), suggesting that it is more accurate at classifying sDAT people.

The RBF kernel SVM, however, has a larger false positive rate since its accuracy is lower (0.6534) than that of the polynomial kernel SVM (0.65). The RBF kernel SVM's specificity (0.8530) is likewise somewhat lower than the polynomial kernel SVM's (0.85), suggesting a greater probability of false negatives.

In terms of accuracy, sensitivity, and balanced accuracy, the RBF kernel SVM outperforms the polynomial and linear SVM models overall, although it has a little worse precision and specificity. As a result, the optimum model to choose will rely on the precise specifications of the categorization problem.

## Final model:-

Finally, leveraging the experience gained from the experiments thus far, we design the “best” SVM classifier for discriminating between the sNC and sDAT groups using the glucose metabolism features derived from the 14 cortical brain regions. We store it as a method named diagnoseDAT.