Assignment 2 – Regression using Scikit-learn

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Git Hub Link. : https://github.com/G-cae78/Regression-Model-Training

Algorithm 1 – Gaussian Process Regression

Detailed Description of Algorithm 1

The Gaussian Processes are nonparametric learning methods which can be used to solve both classification and regression problems. Unlike traditional parametric models which assume a fixed form with a set number of parameters, they can adapt their complexity to the amount of data available to them. The Gaussian process regressor is a supervised learning model described as "Gaussian" because it scales up from finite to an infinite number of dimensions. For any Gaussian process, if any subset of points is picked, those points will follow a multivariate Gaussian distribution which looks like figure 1. The goal of applying these to a dataset is to learn about the underlying distribution. GPs make predictions based on a mean function and a covariance (kernel) function, allowing them to estimate not only the predicted value but also the level of uncertainty associated with each prediction.

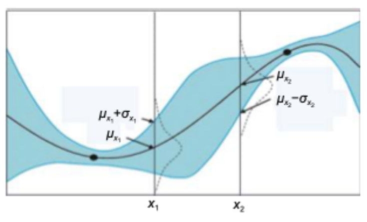


Fig. 1. One-dimensional Gaussian process.

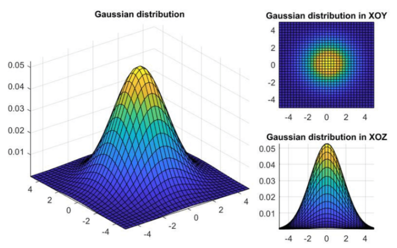


Figure 1 & 2: Shape of a Gaussian Distribution as per ResearchGate and Scikit-Learn (2024)

Why I Chose this Algorithm

GP provides a confidence interval along with its predictions, this would be an invaluable statistic to take into account when finetuning the model, especially in cases where the predictions might not change by much. It's another way to verify the direction each training step is moving in. The size of the dataset also makes it suitable for the GP model, as it is medium-sized and contains 9 features. GP is known to struggle computationally with large datasets but performs really well with smaller to medium-sized ones. Additionally, from looking at the dataset, the relationships between temperature, chemical composition, and tensile strength are most likely smooth and continuous, which aligns with GP's known strength in modelling gradual changes rather than big jumps. Considering the complexity of the chemical combination that determines the final tensile strength, the Gaussian Process would be a perfect fit.

Hyperparameter Details for Tuning.

Kernel : This parameter picks the covariance function of the Gaussian Process. This function defines how data points will influence each other, setting the overall shape smoothness and variability of the learned function. The kernel takes in two points and returns a similarity measure between the points in the form of a scalar. Each kernel is a functional method of its own, taking in its own hyperparameters that control the characteristics and impact the model fit. For example, the WhiteKernel is often combined with other kernels to model observation noise which represents random fluctuations or measurement errors that should not be explained by the underlying function itself. Higher noise levels lead to smoother, more conservative predictions as the GP trats data variations as random noise, while lower noise levels make the model trust the data more closely, potentially leading to overfitting. If no kernel is specified the default is ConstantKernel(1.0, constant_value_bounds="fixed") * RBF(1.0, length_scale_bounds="fixed), which a starting point.

Alpha: The alpha parameter controls stability and tolerance by adding a tiny value to the kernel matrix during training to prevent mathematical errors. Also referred to as nugget, a higher alpha value makes the model ignore small variations and produce smoother predictions; a lower value results in the model following the data more tightly and may increase the risk of overfitting. When used in combination with a kernel such as the WhiteKernel, which already deals with noise, alpha should be kept very small(less than 1e^{-10}) to avoid double-counting the noise in the data.

Algorithm 2 – KNearest Neighbors (KNN) Regression

Detailed Description of Algorithm 2.

KNN is one of many supervised machine learning algorithms. KNN is mostly used for classification tasks, but it also has many benefits when used in regression problems. KNN is often referred to as a *Lazy* Learner because it does not explicitly learn a model during the training phase (GeeksForGeeks, 2025). All of the models' computations, such as measuring the distances between neighbours, are calculated during the prediction. A number of closest data samples, dictated by the k-value, is then selected, and their target values are averaged out to give the final prediction (Scikit-learn, 2024).

KNN is a non-parametric learning method, unlike parametric models that assume a specific form, KNN makes no prior assumptions about the data's distribution before training. It then predicts outcomes based on the similarity between the input data and its closest examples in the training set (Sayed, 2024).

$$\text{distance}(x, X_i) = \sqrt{\sum_{j=1}^{d} (x_j - X_{i_j})^2]} \qquad d\,(x, y) = \sum_{i=1}^{n} |x_i - y_i|$$

$$d\,(x, y) = \left(\sum_{i=1}^{n} (x_i - y_i)^p\right)^{\frac{1}{p}}$$

Figure 3: Mathematical Expressions for Euclidean, Manhattan and Minkowski Distance as per GeeksForGeeks (2025)

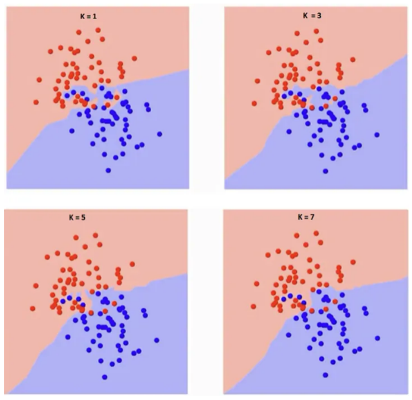


Figure 4: Effects of different K values on a dataset as per (Ebad Sayed on Medium, 2024).

Why I Chose this Algorithm.

KNN's non-parametric feature makes it suitable for the prediction of tensile strength based on the complex and non-linear relationship between temperature and chemical composition. It's simplicity and interpretability will make it easier to understand and visualise the relationships between the parameters and how they interact to determine the final tensile strength of steel. This is particularly useful for identifying patterns and trends within the dataset, providing a good baseline for comparison with more complex regression models like Gaussian Process.

Hyperparameter Details for Tuning.

Metric*:* The metric parameter defines the metric that will be used to compute how close neighbours are within the model. The default distance metric used is the Minkowski, other distance metrics include Euclidean Distance and Manhattan Distance. The Minkowski distance metric generalises to standard Euclidean distance when p=2 (Scikit-learn, 2024). KNN relies on distance metrics to determine which neighbour to use for regression tasks (GeeksForGeeks, 2025). The Euclidean Distance measure the straight line distance from point A to B, while

Manhattan distance is a grid based distance, Minkowski is generally preferred because it serves as a family which encompasses the two other distance metrics (p=2) for Euclidean and (p=1) for Manhattan (GeeksForGeeks, 2025).

N_neighbors: This hyperparameter specifies the number of nearest neighbours to consider when the model is making predictions. The default value for n_neighbors is 5 (Scikit-learn, 2024). For instance, if n_neighbour is set to 5, the algorithm will identify the 5 closest training samples and bases its prediction on the values from those 5 samples. For regression tasks the model typically uses averaging across the data samples to make predict the final value. Smaller values make the model more sensitive to noise and can lead to overfitting, while larger values create smoother boundaries but may oversimplify leading to underfitting (Sayed, 2024). Some approaches used to find the optimal value for this parameter include cross validation which test different values across multiple data splits to find the optimal value that yields the highest accuracy, other methods include elbow method (GeeksForGeeks, 2025).

Algorithm 1 – Gaussian Process Regression - Model Training and Evaluation

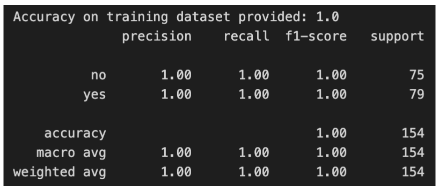
[Todo]

Before training, the entropy was calculated using the entropy( ) function. The result was 0.9995, indicating a lot of irregularities within the data set but also that the dataset is nearly perfectly balanced between both classes, with 51% "yes" and 49% "no" instances. This is advantageous for model training as it minimises the possibility of bias towards one class over another.

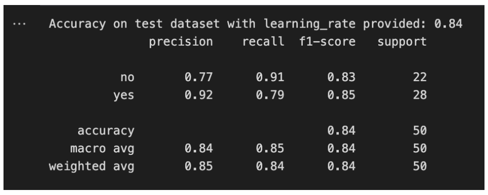
Training and Evaluation Details

[Todo]

The Gradient Boosting algorithm was first trained using its default hyperparameter values of min_samples_leaf=20 and learning_rate = 0.1, and other default parameters as specified in the scikit-learn documentation (Scikit-learn developers, 2024). The model had a strong performance of 100% accuracy and F1-scores across both classes when predicting the training dataset. Although when trying to predict on the test data set there was a dip to only 84% accuracy showing precision of 77% for "no" and 92% for "yes". Result indicates overfitting, a case where the model performs perfectly when predicting the training data because it has memorised it and performs poorer generalising to unseen datasets.



```
Accuracy on training dataset provided: 1.0
              precision    recall  f1-score   support

          no       1.00      1.00      1.00        75
         yes       1.00      1.00      1.00        79

    accuracy                           1.00       154
   macro avg       1.00      1.00      1.00       154
weighted avg       1.00      1.00      1.00       154
```



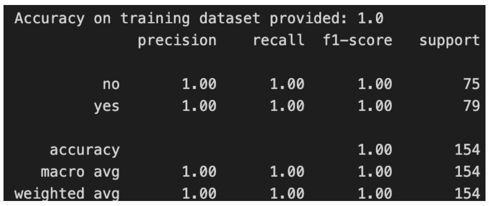
```
... Accuracy on test dataset with learning_rate provided: 0.84
              precision    recall  f1-score   support

          no       0.77      0.91      0.83        22
         yes       0.92      0.79      0.85        28

    accuracy                           0.84        50
   macro avg       0.84      0.85      0.84        50
weighted avg       0.85      0.84      0.84        50
```

Figures 3-4: Model performance with default hyperparameters

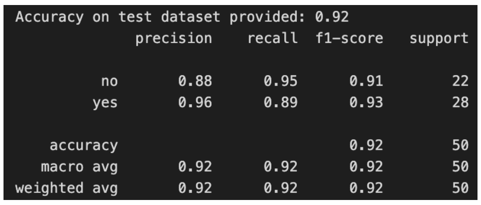
Hyperparameter Tuning

[Todo]

To improve generalisation, the hyperparameters min_samples_leaf and learning_rate were tuned. This tuning involved the manual process of changing the values every run and observing accuracy; this method proved a bit inefficient, although I was able to get it to an accuracy of 90%. With a for-loop I could find the best combination of these hyperparameters and resulting in setting min_samples_leaf = 31 and learning_rate = 0.83 providing greater accuracy of 0.92 on the test dataset whilst still maintaining 100% accuracy on the training dataset.



```
Accuracy on training dataset provided: 1.0
              precision    recall  f1-score   support

          no       1.00      1.00      1.00        75
         yes       1.00      1.00      1.00        79

    accuracy                           1.00       154
   macro avg       1.00      1.00      1.00       154
weighted avg       1.00      1.00      1.00       154
```



```
Accuracy on test dataset provided: 0.92
              precision    recall  f1-score   support

          no       0.88      0.95      0.91        22
         yes       0.96      0.89      0.93        28

    accuracy                           0.92        50
   macro avg       0.92      0.92      0.92        50
weighted avg       0.92      0.92      0.92        50
```

Figures 5-6: Model performance after tuning hyperparameters

Discussion of results

[Todo]

In summary, the tuning process revealed that both hyperparameters significantly influenced model behaviour, improving test performance by 8 percentage points while maintaining training accuracy. Tuning the learning_rate showed that values below 0.5 slowed learning and caused performance to plateau, risking underfitting. For min_samples_leaf, lower values increased model complexity and overfitting risk through more granular splits, while higher values promoted regularisation by restricting splits, thereby improving generalisation on test data.

Algorithm 2 – Nearest Neighbors Regression - Model Training and Evaluation

Training and Evaluation Details

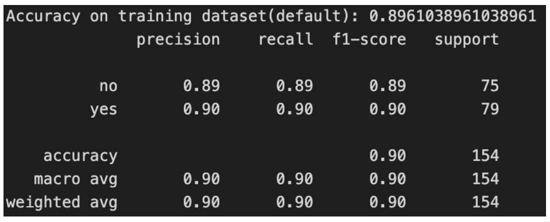
[Todo]

The default parameters for the Logistic Regression can be seen in the scikit-learn developer documentation (Scikit-learn devlopers,2024). It is worth pointing out the default values for the hyper parameters I have chosen to tune; C = 1.0 (regularisation strength) and max_iter = 100 (maximum optimisation iterations).

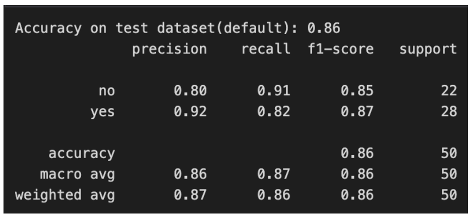
The C value controls the models complexity: higher values will allow the model to fit training data more closely with an increased risk of overfitting, while lower values simplify the model by pernalising large coefficient values reducing overfitting but potentially underfitting. The max_iter parameter determines how many iterations the optimisation algorithm (LBFGS optimiser) has to find the best model coefficients before stopping.

Using the default settings, the model achieved 89.6% accuracy on training data and 86% on test data, showing a 3.6% gap indicating slight overfitting may have occurred. On the test data set, the model showed precision of 0.80 for "no" and 0.92 for "yes", with recall of 0.91 and 0.82, respectively indicating better performance at identifying positive cases but with some false negatives.

The evaluation of default parameter revealed important limitations in the model's optimisation process. During training, the model consistently generated convergence warnings, indicating that the LBFGS optimisation algorithm failed to converge within the default 100 iterations.



```
Accuracy on training dataset(default): 0.8961038961038961
              precision    recall  f1-score   support

          no       0.89      0.89      0.89        75
         yes       0.90      0.90      0.90        79

    accuracy                           0.90       154
   macro avg       0.90      0.90      0.90       154
weighted avg       0.90      0.90      0.90       154
```



```
Accuracy on test dataset(default): 0.86
              precision    recall  f1-score   support

          no       0.80      0.91      0.85        22
         yes       0.92      0.82      0.87        28

    accuracy                           0.86        50
   macro avg       0.86      0.87      0.86        50
weighted avg       0.87      0.86      0.86        50
```

Figure 7-8: LR Model Performance with Default Hyperparameters

Hyperparameter Tuning and Discussion of results

[Todo]

To resolve convergence issues and increase model accuracy and efficiency, max_iter was increased beyond 100. From the training accuracy plot, it can be seen that as C increases and max_iter rises above 200, accuracy steadily improves, eventually exceeding 93% for higher iteration counts. This indicates that additional optimisation steps allow the model to converge and fit the training data closely.

In contrast, the tests accuracy plot shows a clear plateau around 90%, even as C continues to increase. Beyond this point, accuracy begins to fluctuate and decline, indicating overfitting. The model becomes too specialised on the training data, reducing generalisation.

The optimal range for the values was around C = 1=5 and max_iter = 200-400, specifically; C = 4.81 and max_iter = 200, achieving 90% test accuracy and 92% training accuracy. This balances convergence and regularisation without overfitting.

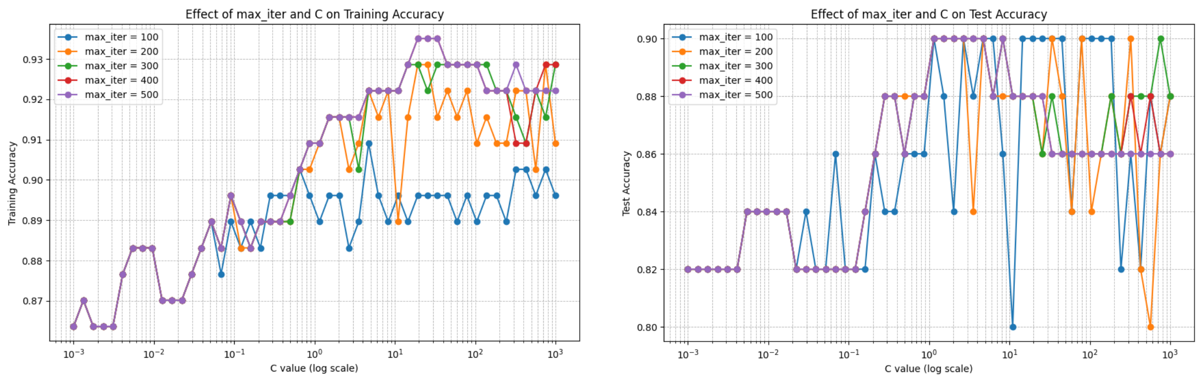


Figure 8-9: Effect of the combination of C-value and Max_iter on model accuracy with test and training data

Comparative Analysis of Algorithm Performances

[Todo]

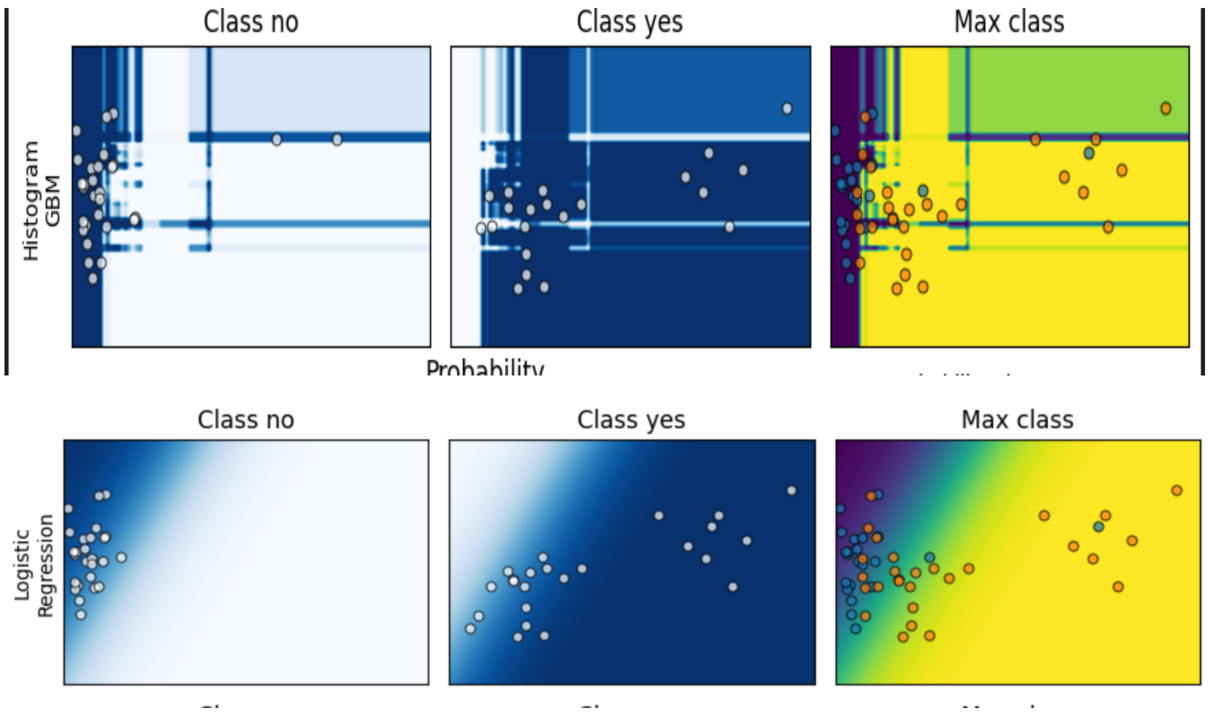


Figure 10 -11: Visualisation of decision boundaries created by both models in 2D projection

From the figures above, we can see how both models learn from the datasets and partition the feature space after learning. Logistic Regression may be limited by its linear pattern forms a straight decision boundary which may struggle to separate more complex data with overlapping patterns. Histogram Based Gradient boosting forms its own decision boundaries piece by piece and is able to adapt flexibly to variations in the dataset. This may explain partly why the Histogram based model performed slightly better than the other due the fact the dataset had a high entropy value (0.995) indicating high levels of irregularities and variations, which may be more suitable to a non-linear model like the Gradient Boosting algorithm.

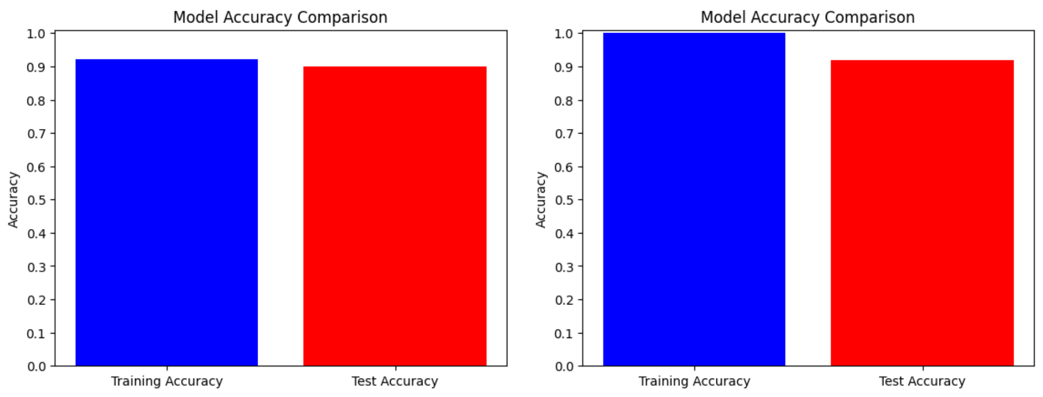


Figure 12 -13: Accuracy results; Logistic Regression(left) and Histogram Based Gradient Boosting(right)

Figures 12 & 13 above compare both models performance. The Histogram-Based Gradient Boosting algorithm performed better on both training and test data sets. The Histogram-based Gradient Boosting achieved 92% accuracy after hyperparameter tuning compared to Logistic Regression's 90%, only a 2% difference. The visualisation of the both models prediction behaviours shows Histogram-based Gradient Boosting produces confident prediction clusters while the plot for Logistic Regression shows a more distributed set of probabilities across ranges. This visualises Histogram-based Gradient Boosting's. ability to learn sharper and develop non-linear decision boundaries compared to Logistic Regression's linear constraints. Although there is a 2% difference in accuracy, it may not be overall

Recommended Hyperparameter Valued based on Results

Gaussian Process Regression (learning_rate): [todo: value]

Gaussian Process Regression (alpha): [todo: value]

Nearest Neighbors Regressor (weights) : [todo: value]

Nearest Neighbors Regressor (n_jobs): [todo: value]

Key Findings

[Todo]

- With the Logistic Regression model, depending on the size of your dataset if you may have to modify the max_iter value to make sure your model can achieve convergence within the number of iterations specified.
- Histogram Based Gradient Boosting uses decision trees underneath but is more efficient due to the binning process, where it splits at boundaries and not at every value. Reducing the amount of data it has to evaluate allows the model to train faster on datasets.
- The decision boundaries of both models differ due to their differences in linearity (see figures 10-11), with Logistic Regression being linear, it produces a smooth and gradual transition between the classes in the decision boundaries. Histogram-based Gradient Boosting on the other hand, is non-linear, leading to more complex and irregular boundaries, which help better capture non-linear patterns within data.

Concluding Remarks

[Todo]

Both models performed well, demonstrating that extensive testing is required to find the optimal combination of the hyperparameters of a model. Given each parameter has trade-offs between efficiency and accuracy that become more complex when combined with others. Overall a fun and good learning exercise.

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Log Of Work

Date	Updates
4/11/25	Research Regression Model
5/11/25	Start Write up for Gaussian Regression
6/11/25	Discuss Hyperparameter selection Finish Write up for Gaussian Process Regression
8/11/25	Research write up fort Voting Regressor
9/11/25	Write about hyperparameters for Voting Regressor Submit half-way point
11/11/25	Redo second algorithm to use KNN instead of voting regressor. Resubmit Half Way point with KNN