Preparation

In [1]:
```
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
from plot_measures import plot_measures
from algorithms_comparison import plot_algorithms_comparison
import warnings
warnings.filterwarnings('ignore')
```

Introduction

The purpose of this project is to implement a logistic model from scratch and to test the performance of different optimisation algorithms. We begin with preparing the data for analysis, then we implement 3 optimization algorithms for training the model, and finally we assess the result using statistical measures.

Datasets

Since the model needs to be trained and tested, there is a need to prepare some data. We collected 5 datasets:

- **candies** - dataset concerning production of candies. Sample questions addressed by the variables: *Does it contain chocolate?, Is it fruit flavored?, Is there caramel in the candy?, Does it contain peanuts, peanut butter or almonds?, Does it contain nougat?*. The target variable describes percentage of people who liked this candie type.
- **breast cancer** - dataset describing health state of a patients suffering from breast cancer. The target variable describes if the cancer is maligant.
- **bankrupcy** - this is a dataset from a recruiting task from a consulting firm. Variables include information of each candidating company, for example income, marketing statistics, ratings, sector number of employees, etc. The target variable represents information about bankrupcy. This dataset is significantly larger than other.
- **nba** - dataset on all the NBA finals results and NBA Regular Seasons MVP.
- **wine** - dataset related to red and white variants of the Portuguese "Vinho Verde" wine.

The first step was downloading the data and conversion of types. We saved the initially preprocessed data under directory `data/before preprocessing`. Next step was to replace missing data with mean value of each variable. Then we analyzed correlation matric for each dataset and we dropped the most correlated variables.

Measures

We introduce 3 measures of fit: *accuracy*, *precission* and *recall*. The implementation can be found in `log_regression.py` file.

$$accuracy(y, \hat{y}) = \frac{1}{n} \sum_{i} I_{\left\{y_i = \hat{y}_i\right\}}$$

$$precision(y, \hat{y}) = \frac{\sum_i I_{\{y_i = \hat{y}_i = 1\}}}{\sum_i I_{\{\hat{y}_i = 1\}}}$$

$$recall(y, \hat{y}) = \frac{\sum_i I_{\{y_i = \hat{y}_i = 1\}}}{\sum_i I_{\{y_i = 1\}}}$$

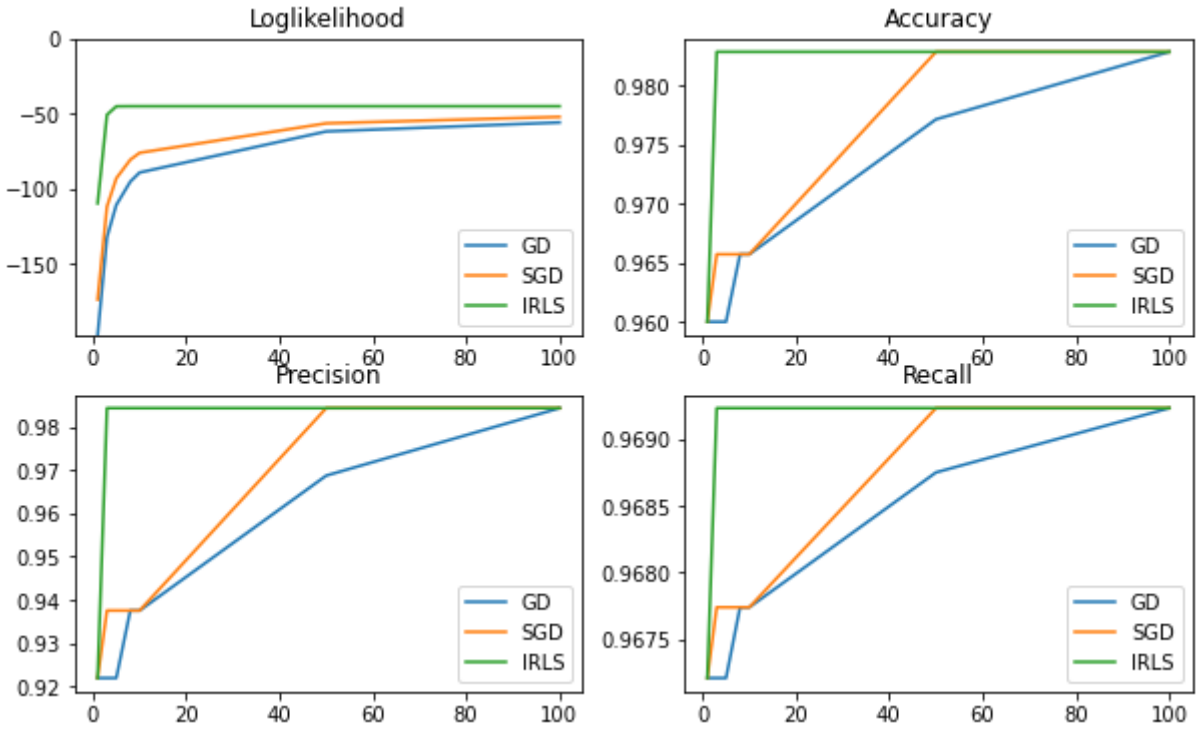
Model

The main component of our model is the `LogisticModel` class present in `log_regression.py` file. It includes 3 training methods - `GD`, `SGD` and `IRLS`, method `fit` which given a dataset predicts the results and measures like `log_likelihood` and `R2_measure`.

Loglikelihood and goodness of fit

We have examined how loglikelihood and other measures are affected by number of iterations. Increasing number of iterations makes a difference mainly for smaller number of iterations.

In [4]:
```
plot_measures()
```



Stopping Rule

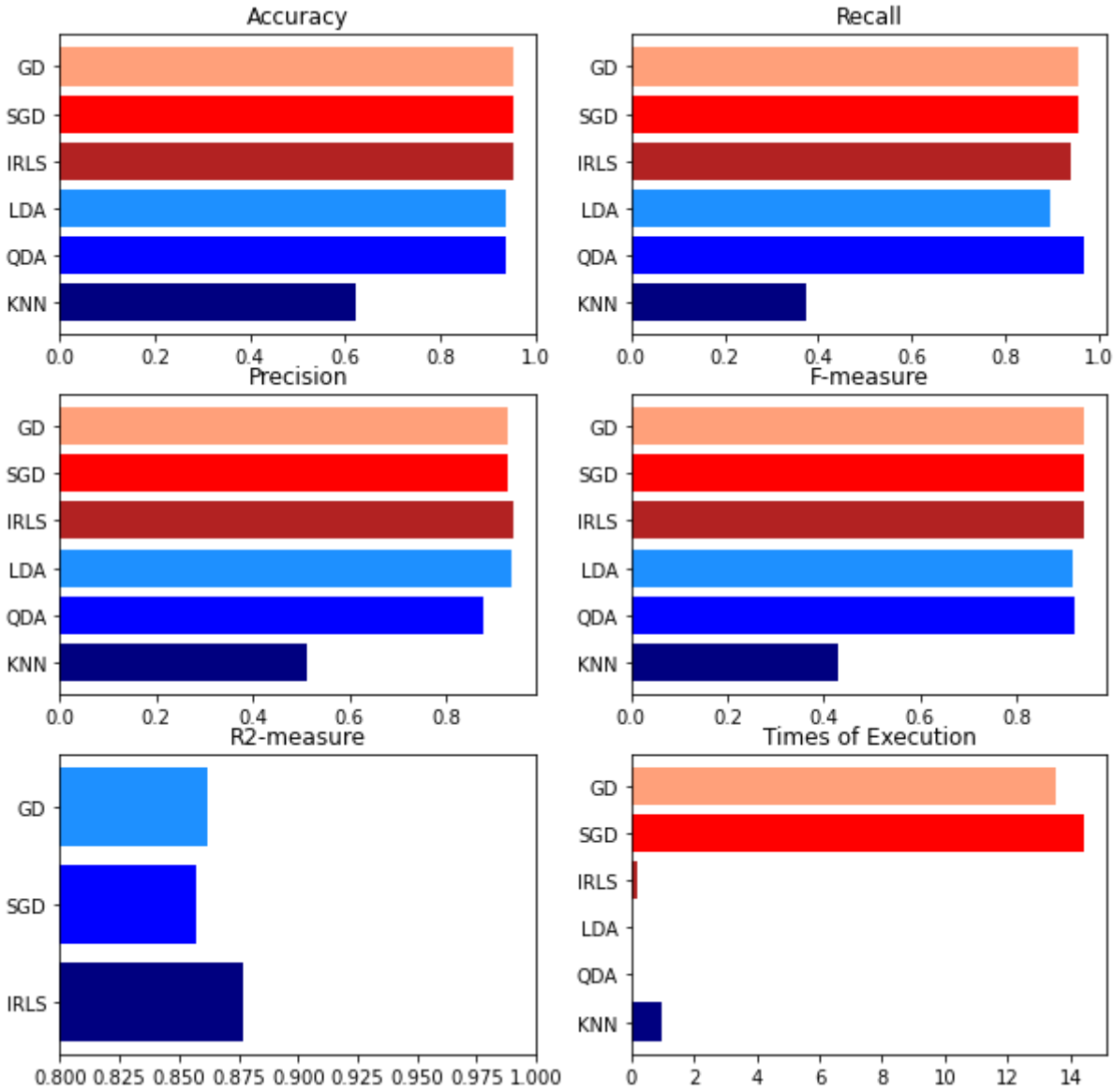
Several different methods of stopping rules for the algorithms are possible, but we decided to choose one of the most universal ones which is also used for training neural networks such as *Multilayer Perceptron*. Each algorithm was started with a vector of weights consisting only zeros (this approach also helped **IRLS** converge more effectively). In each iteration of the algorithm, we compared the new weights with the previous ones by calculating the norm of the difference of weights vectors. With previously assigned *epsilon*, we checked if the norm is less than the *epsilon*. If that was the case, we stopped the algorithm printing the number of iterations.

$$\|w_{n+1} - w_n\| < \epsilon, \quad \text{where } n+1 \text{ is the number of current iteration.}$$

Comparison With Other Classification Algorithms

We compared the logistic model created by us (concerning all the implemented optiomization algorithms) againts other popular models, like LDA, QDA and KNN. We used the **breast cancer** for the computation. Below we present the results of the comparison:

In [5]:
```
plot_algorithms_comparison(figsize=(10, 10))
```



Note that the first 4 measures are pretty similar for **GD**, **SGD**, **IRLS**, and **LDA**. **QDA** seems to perform slightly worse on this dataset, while **KNN** has the worst results. This might be caused by high dimensionality of the data. We can also see that **IRLS** reaches the highest *R2 measure*, while both **GD** and **SGD** are again very similar.

Times of execution for the first 3 algorithms may prove to be significantly higher, because these algorithms were implemented using only basic functions from *numpy* module. Although **IRLS** uses algorithm of calculating pseudo-inverse/inverse matrix, its time of execution appears to be significantly slower in comparison with **GD** and **SGD**.

For **KNN** algorithm, we used very basic optimization for choosing the most accurate *k* by checking accuracies of the model for different values from range 1 to 50. This might have

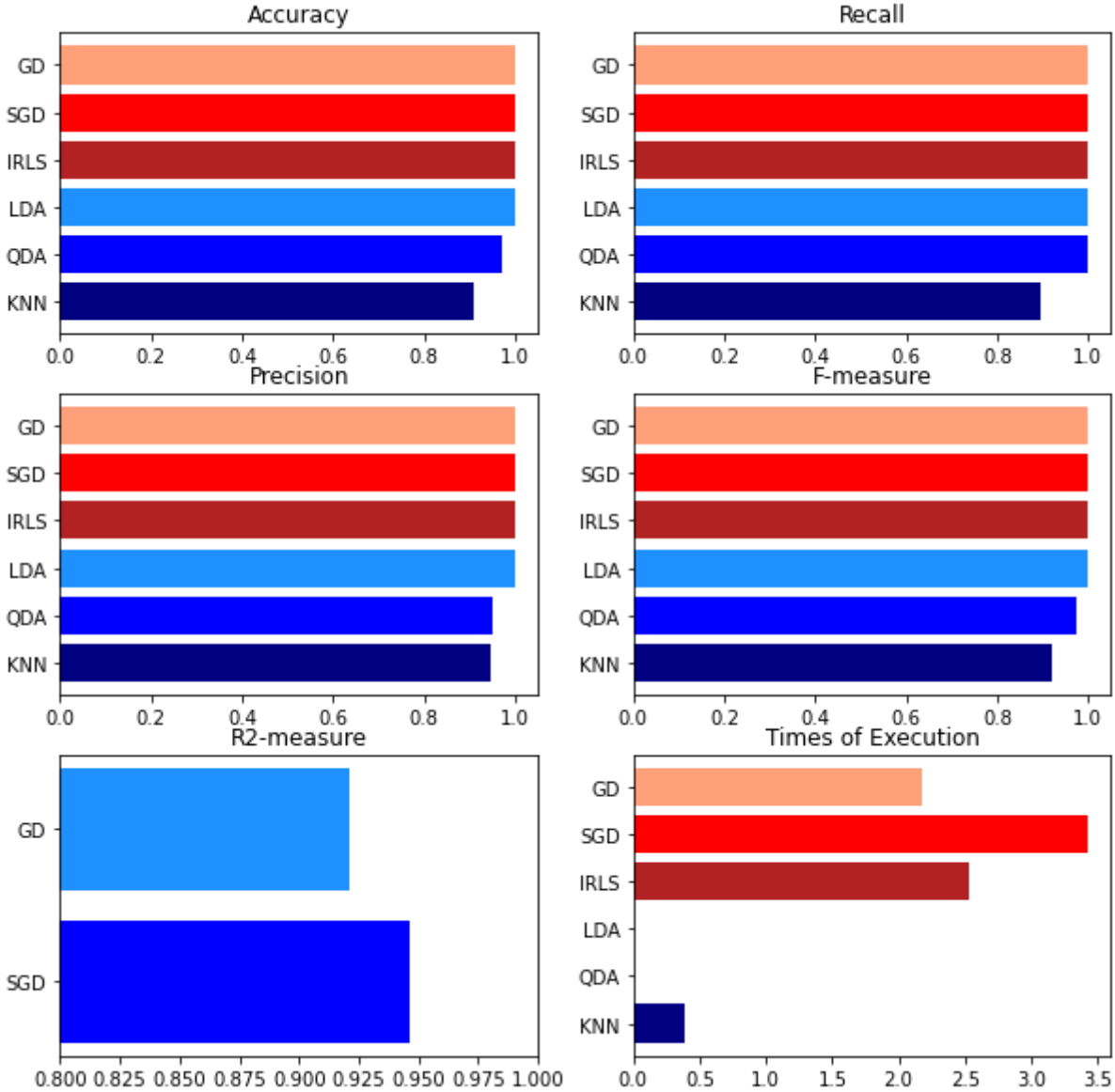
slowed the execution of this classification algorithm.

We would like to also mention the method for calculating the *R2 measure*. To calculate this measure, we prepared the *null model* for the given learning data. It is a model that consists only the intercept. We treated such a model as a typical logistic regression model with the weights equal to *0* except for the intercept.

$$\ln \frac{\pi}{1-\pi} = \beta_0, \quad \text{where } \pi = \mathbb{P}(Y = 1).$$

Therefore, the only non-zero weight was calculated as a natural logarithm of the odds of belonging to class *1*. We estimated the probability of belonging to this class by calculating the average value of *Y*-variable.

In [6]:
```
dataset = pd.read_csv(f"data/after preprocessing/wine.csv")
target_name = "Target"
plot_algorithms_comparison(dataset, target_name, figsize=(10, 10))
```



Once we tested the algorithms on different datasets, we noticed that sometimes **IRLS** converges to weights that make activation function be equal exactly to *0* or *1*. This behaviour made it impossible to calculate the logarithm of likelihood function and consequently, we were unable to calculate the *R2 measure* for such models.

Using **IRLS** algorithm for optimization sometimes resulted in obtaining singular matrix that was intended to be inversed. We thought of two approaches:

- checking if the matrix appears to be singular, stopping the algorithm, and using the most recent weights
- calculating the Moore-Penrose pseudo-inverse of a matrix using its singular-value decomposition (SVD) which is a generalisation of the inverse.

We decided to follow the second approach and the results were satisfying for IRLS based on the above plots.