

# Thesis Simulation Single Run for Chapter 4

Dasha Asienga

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## Contents

<b>Logistic Regression</b>	<b>1</b>
Reading in the Data . . . . .	1
Fitting the Logistic Regression . . . . .	1
Convergence . . . . .	2
Accuracy . . . . .	2
Discrimination . . . . .	2
<b>Seldonian Framework</b>	<b>3</b>
Reading in the Data . . . . .	3
Pre-Processing the Data . . . . .	3
Fitting a Seldonian Algorithm . . . . .	4
Convergence . . . . .	7
Accuracy . . . . .	8
Discrimination . . . . .	10
<b>Results</b>	<b>13</b>
<b>Note</b>	<b>14</b>

This file is intended to run the simulation process on the parent simulation data set as a single run, before scaling it into multiple trials.

## Logistic Regression

### Reading in the Data

First, let's read in the parent simulation data set.

```
compas_sim_path <- "/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/compas_sim.csv"
compas_sim_parent <- read.csv(compas_sim_path)
```

### Fitting the Logistic Regression

We'll want to run the logistic regression as our baseline model and obtain the 3 key performance measures: convergence, accuracy, and discrimination.

```
lr <- glm(is_recid ~ age + prior_offense,
          data = compas_sim_parent,
          family = binomial(logit))
```

## Convergence

Obtain convergence as an object. We would expect LR to always converge.

```
lr_converged <- lr[["converged"]]  
lr_converged
```

```
## [1] TRUE
```

## Accuracy

Conditional on convergence, obtain the accuracy as an object, which in this case is 60.76%.

```
lr_accuracy <- count(round(lr[["fitted.values"]]) == lr[["y"]]) / nrow(compas_sim_parent)  
lr_accuracy
```

```
## n_TRUE  
## 0.6076
```

## Discrimination

Conditional on convergence, obtain the discrimination statistic as an object, which in this case is 0.2784 or 27.84%.

```
preds <- predict(lr, newdata = compas_sim_parent, type="response")  
  
compas_sim_parent <- compas_sim_parent %>%  
  mutate(preds = preds,  
         prediction = round(preds, 0),  
         pred_risk = ifelse(prediction == 0, 'Low', 'High'))  
  
discrimination <- compas_sim_parent %>%  
  dplyr::select(race, pred_risk, is_recid) %>%  
  group_by(race, is_recid) %>%  
  mutate(total = n()) %>%  
  group_by(pred_risk, race, total) %>%  
  summarise("reoffended" = count(is_recid == 1),  
            "did_not_reoffend" = count(is_recid == 0)) %>%  
  pivot_longer(cols = c("reoffended", "did_not_reoffend"),  
              names_to = "recidivism") %>%  
  pivot_wider(  
    id_cols = c("pred_risk", "recidivism", "total"),  
    names_from = "race",  
    values_from = value  
  ) %>%  
  rename("Black" = `African-American`,  
         "White" = `Caucasian`) %>%  
  mutate(Black = round(100 * Black / total, 2),
```

```

        White = round(100 * White / total, 2)) %>%
dplyr::select(-total) %>%
group_by(pred_risk, recidivism) %>%
summarize(Black = max(Black, na.rm = TRUE),
          White = max(White, na.rm = TRUE)) %>%
filter((pred_risk == "High" & recidivism == "did_not_reoffend") |
       (pred_risk == "Low" & recidivism == "reoffended"))
)

lr_disc_stat <- sum(abs(discrimination$White - discrimination$Black))/100
lr_disc_stat

## [1] 0.2784

```

The results from the logistic regression are now easily savable and retrievable, which will be useful when we scale the process.

## Seldonian Framework

We also want to be able to easily retrieve the 3 key performance measures from the Seldonian algorithms we run before we scale the process, that is, convergence, accuracy, and discrimination.

### Reading in the Data

First, let's read in the data.

```

# point to the data file
f_orig = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/compas_sim.csv"

columns_orig = ["race", "prior_offense", "age", "is_recid"]

df = pd.read_csv(f_orig, header=0, names=columns_orig)

```

### Pre-Processing the Data

Let's also preprocess the data to prepare it for Seldonian modeling.

```

# select inputs to be transformed
X = df.drop(columns=["is_recid"])
y = df["is_recid"]

# one hot encode race, scale age using standard scaler
ct = ColumnTransformer([('c', OneHotEncoder(), ['race']), ('n', StandardScaler(), ['age'])])

# apply transformation
X_transformed = ct.fit_transform(X)

# get names after one-hot encoding
output_columns = ct.get_feature_names_out(ct.feature_names_in_)

# make an output dataframe to save transformed X and y
outdf = pd.DataFrame(X_transformed, columns=output_columns)

```

```

# change names of columns
outdf.rename(columns={'c__race_African-American':'Black', 'c__race_Caucasian':'White', 'n__age':'age'},

# re-index in order to concatenate columns
prior_offense = df["prior_offense"]
y.index = range(0, len(y))
prior_offense.index = range(0, len(prior_offense))

# add label column and `prior_offense` into final dataframe
outdf['prior_offense'] = prior_offense
outdf['is_recid'] = y

```

The data set is now clean and ready. Let's save it along with the JSON metadata file.

```

# save final dataframe
output_path_data="/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/Simulation Single Run"

outdf.to_csv(output_path_data,index=False,header=False)

# save metadata json file
output_path_metadata="/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/Simulation Single Run"

metadata_dict = {
    "regime":"supervised_learning",
    "sub_regime":"classification",
    "all_col_names":list(outdf.columns),
    "label_col_names":"is_recid",
    "sensitive_col_names":["Black", "White"]
}

with open(output_path_metadata,'w') as outfile:
    json.dump(metadata_dict,outfile,indent=2)

```

## Fitting a Seldonian Algorithm

Varying  $\epsilon = 0.2, 0.1, 0.05$ , &  $0.01$ , let's fit a Seldonian algorithm such that

$$abs((FNR|[Black]) - (FNR|[White])) + abs((FPR|[Black]) - (FPR|[White])) \leq \epsilon.$$

We will take  $\delta = 0.05$  to ensure 95% confidence.

First, let's read in the data set and specify the regime.

```

import autograd.numpy as np

data_pth = output_path_data
metadata_pth = output_path_metadata
save_dir = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/"
os.makedirs(save_dir,exist_ok=True)

# create dataset from data and metadata file

```

```

regime='supervised_learning'
sub_regime='classification'

loader = DataSetLoader(regime=regime)

dataset = loader.load_supervised_dataset(
    filename=data_pth,
    metadata_filename=metadata_pth,
    file_type='csv')

sensitive_col_names = dataset.meta.sensitive_col_names

# use logistic regression model
model = LogisticRegressionModel()

# set the primary objective to be log loss
primary_objective = objectives.binary_logistic_loss

```

Next, let's create and save the specification files for each of the four levels of  $\epsilon$ .

```

from seldonian.spec import createSupervisedSpec

# define behavioral constraints (epsilon = 0.2)
epsilon = 0.2
constraint_name = "equalized_odds"
if constraint_name == "equalized_odds":
    constraint_strs = [f'abs((FNR | [Black]) - (FNR | [White])) + abs((FPR | [Black]) - (FPR | [White])) < {epsilon}']
    deltas = [0.05]

# create spec file
save_dir = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equalized_odds_epsilon_0.2"

os.makedirs(save_dir, exist_ok=True) #create folder

createSupervisedSpec(
    dataset=dataset,
    metadata_pth=metadata_pth,
    constraint_strs=constraint_strs,
    deltas=deltas,
    save_dir=save_dir,
    save=True,
    verbose=False)

```

```
## <seldonian.spec.SupervisedSpec object at 0x7ffe8e022e10>
```

```

#-----#

# define behavioral constraints (epsilon = 0.1)
epsilon = 0.1
constraint_name = "equalized_odds"
if constraint_name == "equalized_odds":
    constraint_strs = [f'abs((FNR | [Black]) - (FNR | [White])) + abs((FPR | [Black]) - (FPR | [White])) < {epsilon}']

```

```

deltas = [0.05]

# create spec file
save_dir = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali

os.makedirs(save_dir, exist_ok=True) #create folder

createSupervisedSpec(
    dataset=dataset,
    metadata_pth=metadata_pth,
    constraint_strs=constraint_strs,
    deltas=deltas,
    save_dir=save_dir,
    save=True,
    verbose=False)

```

```
## <seldonian.spec.SupervisedSpec object at 0x7ffe8d7f3510>
```

```

#-----#

# define behavioral constraints (epsilon = 0.05)
epsilon = 0.05
constraint_name = "equalized_odds"
if constraint_name == "equalized_odds":
    constraint_strs = [f'abs((FNR | [Black]) - (FNR | [White])) + abs((FPR | [Black]) - (FPR | [White]))'
    deltas = [0.05]

# create spec file
save_dir = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali

os.makedirs(save_dir, exist_ok=True) #create folder

createSupervisedSpec(
    dataset=dataset,
    metadata_pth=metadata_pth,
    constraint_strs=constraint_strs,
    deltas=deltas,
    save_dir=save_dir,
    save=True,
    verbose=False)

```

```
## <seldonian.spec.SupervisedSpec object at 0x7ffe8d8c2510>
```

```

#-----#

# define behavioral constraints (epsilon = 0.01)
epsilon = 0.01
constraint_name = "equalized_odds"
if constraint_name == "equalized_odds":
    constraint_strs = [f'abs((FNR | [Black]) - (FNR | [White])) + abs((FPR | [Black]) - (FPR | [White]))'
    deltas = [0.05]

# create spec file
save_dir = "/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali

```

```
os.makedirs(save_dir, exist_ok=True) #create folder
```

```
createSupervisedSpec(  
    dataset=dataset,  
    metadata_pth=metadata_pth,  
    constraint_strs=constraint_strs,  
    deltas=deltas,  
    save_dir=save_dir,  
    save=True,  
    verbose=False)
```

```
## <seldonian.spec.SupervisedSpec object at 0x7ffe8d7f1310>
```

Finally, let's run the Seldonian engine for each of the four specification files.

```
from seldonian.seldonian_algorithm import SeldonianAlgorithm  
from seldonian.utils.io_utils import load_pickle
```

```
# load the spec file (epsilon = 0.2)
```

```
specfile = '/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali
```

```
spec = load_pickle(specfile)
```

```
SA_02 = SeldonianAlgorithm(spec)
```

```
#-----#
```

```
# load the spec file (epsilon = 0.1)
```

```
specfile = '/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali
```

```
spec = load_pickle(specfile)
```

```
SA_01 = SeldonianAlgorithm(spec)
```

```
#-----#
```

```
# load the spec file (epsilon = 0.05)
```

```
specfile = '/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali
```

```
spec = load_pickle(specfile)
```

```
SA_005 = SeldonianAlgorithm(spec)
```

```
#-----#
```

```
# load the spec file (epsilon = 0.01)
```

```
specfile = '/home/dasienga24/Statistics-Senior-Honors-Thesis/Python/COMPAS Simulation/Single Run/equali
```

```
spec = load_pickle(specfile)
```

```
SA_001 = SeldonianAlgorithm(spec)
```

## Convergence

Obtain and store convergence as an object.

**epsilon = 0.2**

```
passed_safety_02, solution_02 = SA_02.run(write_cs_logfile=True)  
passed_safety_02
```

```
## True
```

```
epsilon = 0.1
```

```
passed_safety_01, solution_01 = SA_01.run(write_cs_logfile=True)
passed_safety_01
```

```
## True
```

```
epsilon = 0.05
```

```
passed_safety_005, solution_005 = SA_005.run(write_cs_logfile=True)
passed_safety_005
```

```
## True
```

```
epsilon = 0.01
```

```
passed_safety_001, solution_001 = SA_001.run(write_cs_logfile=True)
passed_safety_001
```

```
## True
```

## Accuracy

Obtain and store accuracy as an object.

```
# separate the predictor variables from the sensitive variable and the response variable
X_outdf = outdf.drop(columns = ['is_recid', 'Black', 'White'])
X_sens = outdf[['Black', 'White']]
y_outdf = outdf['is_recid']
```

```
#-----#
# get the solution & store coefficients (epsilon = 0.2)
coefficients = SA_02.cs_result["candidate_solution"]
```

```
# get the intercept
intercept = coefficients[0]
```

```
# compute the predictive values
linear_combination = np.dot(X_outdf, coefficients[1:]) + intercept
pred_probs_02 = 1 / (1 + np.exp(-linear_combination))
```

```
#-----#
# get the solution & store coefficients (epsilon = 0.1)
coefficients = SA_01.cs_result["candidate_solution"]
```

```
# get the intercept
intercept = coefficients[0]
```

```
# compute the predictive values
linear_combination = np.dot(X_outdf, coefficients[1:]) + intercept
pred_probs_01 = 1 / (1 + np.exp(-linear_combination))
```



```

#-----#
# get the solution & store coefficients (epsilon = 0.05)
coefficients = SA_005.cs_result["candidate_solution"]

# get the intercept
intercept = coefficients[0]

# compute the predictive values
linear_combination = np.dot(X_outdf, coefficients[1:]) + intercept
pred_probs_005 = 1 / (1 + np.exp(-linear_combination))

#-----#
# get the solution & store coefficients (epsilon = 0.01)
coefficients = SA_001.cs_result["candidate_solution"]

# get the intercept
intercept = coefficients[0]

# compute the predictive values
linear_combination = np.dot(X_outdf, coefficients[1:]) + intercept
pred_probs_001 = 1 / (1 + np.exp(-linear_combination))

# store results
seldonian_results = pd.DataFrame({'is_recid': y_outdf, 'pred_0.2': pred_probs_02, 'pred_0.1': pred_probs_01, 'pred_0.05': pred_probs_005, 'pred_0.01': pred_probs_001})
seldonian_results = pd.concat([X_outdf, X_sens, seldonian_results], axis = 1)

# define threshold
threshold = 0.5

# create risk columns
risk_02 = np.where(pred_probs_02 >= threshold, 1, 0)
risk_01 = np.where(pred_probs_01 >= threshold, 1, 0)
risk_005 = np.where(pred_probs_005 >= threshold, 1, 0)
risk_001 = np.where(pred_probs_001 >= threshold, 1, 0)

# add risk columns to dataframe
seldonian_results['risk_0.2'] = risk_02
seldonian_results['risk_0.1'] = risk_01
seldonian_results['risk_0.05'] = risk_005
seldonian_results['risk_0.01'] = risk_001

# write the dataframe to a CSV file
seldonian_results.to_csv("/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/Simulation Results/seldonian_results.csv")

# read in the data
seldonian_results <- read.csv("/home/dasienga24/Statistics-Senior-Honors-Thesis/Data Sets/COMPAS/Simulation Results/seldonian_results.csv")

epsilon = 0.2

sa_0.2_accuracy <- count(seldonian_results$risk_0.2 == seldonian_results$is_recid)/nrow(seldonian_results)
sa_0.2_accuracy

## n_TRUE

```

```
## 0.611
```

```
epsilon = 0.1
```

```
sa_0.1_accuracy <- count(seldonian_results$risk_0.1 == seldonian_results$is_recid)/nrow(seldonian_resul  
sa_0.1_accuracy
```

```
## n_TRUE
```

```
## 0.6124
```

```
epsilon = 0.05
```

```
sa_0.05_accuracy <- count(seldonian_results$risk_0.05 == seldonian_results$is_recid)/nrow(seldonian_res  
sa_0.05_accuracy
```

```
## n_TRUE
```

```
## 0.609
```

```
epsilon = 0.01
```

```
sa_0.01_accuracy <- count(seldonian_results$risk_0.01 == seldonian_results$is_recid)/nrow(seldonian_res  
sa_0.01_accuracy
```

```
## n_TRUE
```

```
## 0.5092
```

## Discrimination

Obtain and store the discrimination statistic as an object.

```
seldonian_results <- seldonian_results %>%  
  mutate(race = ifelse(Black == 1, 'Black', 'White'),  
         pred_risk_0.2 = ifelse(risk_0.2 == 0, 'Low', 'High'),  
         pred_risk_0.1 = ifelse(risk_0.1 == 0, 'Low', 'High'),  
         pred_risk_0.05 = ifelse(risk_0.05 == 0, 'Low', 'High'),  
         pred_risk_0.01 = ifelse(risk_0.01 == 0, 'Low', 'High'))
```

```
epsilon = 0.2
```

```
discrimination <- seldonian_results %>%  
  dplyr::select(race, pred_risk_0.2, is_recid) %>%  
  group_by(race, is_recid) %>%  
  mutate(total = n()) %>%  
  group_by(pred_risk_0.2, race, total) %>%  
  summarise("reoffended" = count(is_recid == 1),  
           "did_not_reoffend" = count(is_recid == 0)) %>%  
  pivot_longer(cols = c("reoffended", "did_not_reoffend"),  
              names_to = "recidivism") %>%  
  pivot_wider(  
    id_cols = c("pred_risk_0.2", "recidivism", "total"),  
    names_from = "race",  
    values_from = value  
  ) %>%  
  mutate(Black = round(100 * Black / total, 2),
```

```

        White = round(100 * White / total, 2)) %>%
dplyr::select(-total) %>%
group_by(pred_risk_0.2, recidivism) %>%
summarize(Black = max(Black, na.rm = TRUE),
          White = max(White, na.rm = TRUE)) %>%
filter((pred_risk_0.2 == "High" & recidivism == "did_not_reoffend") |
       (pred_risk_0.2 == "Low" & recidivism == "reoffended")
)

sa_0.2_disc_stat <- sum(abs(discrimination$White - discrimination$Black))/100
sa_0.2_disc_stat

```

```
## [1] 0.276
```

epsilon = 0.1

```

discrimination <- seldonian_results %>%
dplyr::select(race, pred_risk_0.1, is_recid) %>%
group_by(race, is_recid) %>%
mutate(total = n()) %>%
group_by(pred_risk_0.1, race, total) %>%
summarise("reoffended" = count(is_recid == 1),
          "did_not_reoffend" = count(is_recid == 0)) %>%
pivot_longer(cols = c("reoffended", "did_not_reoffend"),
             names_to = "recidivism") %>%
pivot_wider(
  id_cols = c("pred_risk_0.1", "recidivism", "total"),
  names_from = "race",
  values_from = value
) %>%
mutate(Black = round(100 * Black / total, 2),
       White = round(100 * White / total, 2)) %>%
dplyr::select(-total) %>%
group_by(pred_risk_0.1, recidivism) %>%
summarize(Black = max(Black, na.rm = TRUE),
          White = max(White, na.rm = TRUE)) %>%
filter((pred_risk_0.1 == "High" & recidivism == "did_not_reoffend") |
       (pred_risk_0.1 == "Low" & recidivism == "reoffended")
)

sa_0.1_disc_stat <- sum(abs(discrimination$White - discrimination$Black))/100
sa_0.1_disc_stat

```

```
## [1] 0.2176
```

epsilon = 0.05

```

discrimination <- seldonian_results %>%
dplyr::select(race, pred_risk_0.05, is_recid) %>%
group_by(race, is_recid) %>%
mutate(total = n()) %>%
group_by(pred_risk_0.05, race, total) %>%
summarise("reoffended" = count(is_recid == 1),
          "did_not_reoffend" = count(is_recid == 0)) %>%

```

```

pivot_longer(cols = c("reoffended", "did_not_reoffend"),
             names_to = "recidivism") %>%
pivot_wider(
  id_cols = c("pred_risk_0.05", "recidivism", "total"),
  names_from = "race",
  values_from = value
) %>%
mutate(Black = round(100 * Black / total, 2),
       White = round(100 * White / total, 2)) %>%
dplyr::select(-total) %>%
group_by(pred_risk_0.05, recidivism) %>%
summarize(Black = max(Black, na.rm = TRUE),
          White = max(White, na.rm = TRUE)) %>%
filter((pred_risk_0.05 == "High" & recidivism == "did_not_reoffend") |
       (pred_risk_0.05 == "Low" & recidivism == "reoffended"))
)

sa_0.05_disc_stat <- sum(abs(discrimination$White - discrimination$Black))/100
sa_0.05_disc_stat

```

```
## [1] 0.2072
```

epsilon = 0.01

```

discrimination <- seldonian_results %>%
  dplyr::select(race, pred_risk_0.01, is_recid) %>%
  group_by(race, is_recid) %>%
  mutate(total = n()) %>%
  group_by(pred_risk_0.01, race, total) %>%
  summarise("reoffended" = count(is_recid == 1),
            "did_not_reoffend" = count(is_recid == 0)) %>%
  pivot_longer(cols = c("reoffended", "did_not_reoffend"),
               names_to = "recidivism") %>%
  pivot_wider(
    id_cols = c("pred_risk_0.01", "recidivism", "total"),
    names_from = "race",
    values_from = value
  ) %>%
  mutate(Black = round(100 * Black / total, 2),
         White = round(100 * White / total, 2)) %>%
  dplyr::select(-total) %>%
  group_by(pred_risk_0.01, recidivism) %>%
  summarize(Black = max(Black, na.rm = TRUE),
            White = max(White, na.rm = TRUE)) %>%
  filter((pred_risk_0.01 == "High" & recidivism == "did_not_reoffend") |
         (pred_risk_0.01 == "Low" & recidivism == "reoffended"))
  )

sa_0.01_disc_stat <- sum(abs(discrimination$White - discrimination$Black))/100
sa_0.01_disc_stat

```

```
## [1] 0.0608
```

## Results

Synthesize results for reporting.

```
# create a vector of accuracies
accuracy_vector <- c(lr_accuracy, sa_0.2_accuracy, sa_0.1_accuracy, sa_0.05_accuracy, sa_0.01_accuracy)

# transpose the vector to create a data frame with 5 columns
accuracy_df <- as.data.frame(t(accuracy_vector))

# name the columns of the data frame
colnames(accuracy_df) <- c("LR", "SA (0.2)", "SA (0.1)", "SA (0.05)", "SA (0.01)")

accuracy_df %>%
  kable(caption = "Model Accuracy")
```

Table 1: Model Accuracy

LR	SA (0.2)	SA (0.1)	SA (0.05)	SA (0.01)
0.6076	0.611	0.6124	0.609	0.5092

```
# create a vector of discrimination
disc_vector <- c(lr_disc_stat, sa_0.2_disc_stat, sa_0.1_disc_stat, sa_0.05_disc_stat, sa_0.01_disc_stat)

# transpose the vector to create a data frame with 5 columns
disc_df <- as.data.frame(t(disc_vector))

# name the columns of the data frame
colnames(disc_df) <- c("LR", "SA (0.2)", "SA (0.1)", "SA (0.05)", "SA (0.01)")

disc_df %>%
  kable(caption = "Model Discrimination")
```

Table 2: Model Discrimination

LR	SA (0.2)	SA (0.1)	SA (0.05)	SA (0.01)
0.2784	0.276	0.2176	0.2072	0.0608

```
plot_data <- accuracy_df %>%
  union(disc_df) %>%
  pivot_longer(cols = c("LR", "SA (0.2)", "SA (0.1)", "SA (0.05)", "SA (0.01)"),
    names_to = "model", values_to = "value") %>%
  mutate(statistic = ifelse(row_number() <= 5, "accuracy", "discrimination"))

# define the desired order of the x-axis
desired_order <- c("LR", "SA (0.2)", "SA (0.1)", "SA (0.05)", "SA (0.01)")

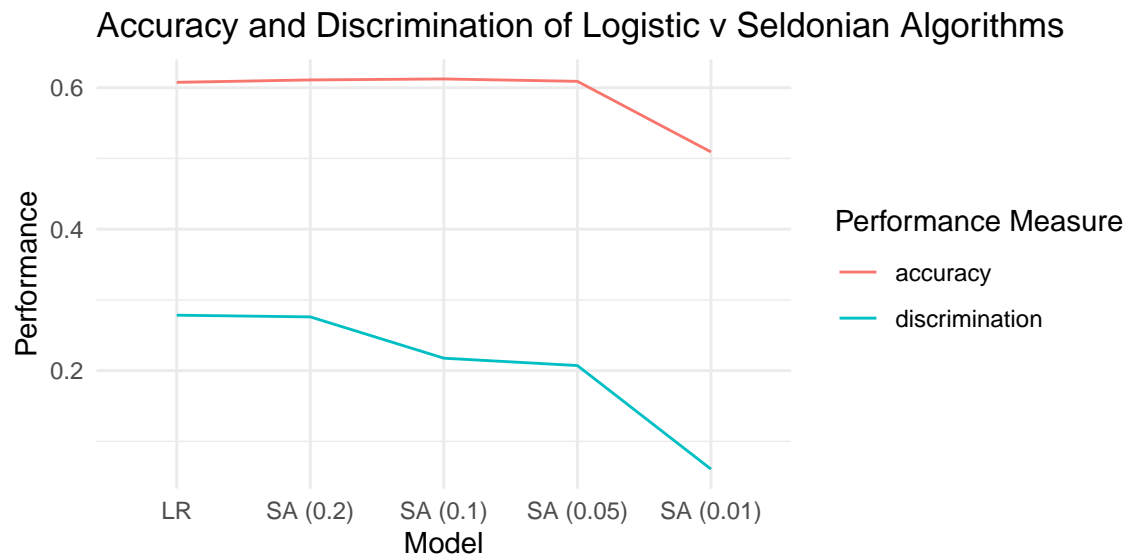
# convert the 'model' variable to a factor with the desired order
plot_data$model <- factor(plot_data$model, levels = desired_order)

# plot
ggplot(data = plot_data, mapping = aes(x = model,
```

```

y = value,
color = statistic,
group = statistic)) +
geom_line() +
theme_minimal() +
labs(x = "Model",
     y = "Performance",
     color = "Performance Measure",
     title = "Accuracy and Discrimination of Logistic v Seldonian Algorithms")

```



## Note

Before scaling this process, I will need to separately handle and track instances where the Seldonian algorithm does not converge, in case such cases emerge.