Rtificial intelligence

A guide to using R for ML

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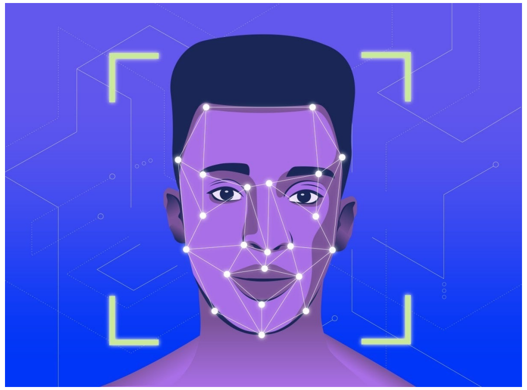
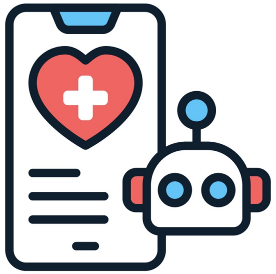
06-22-2024

Cascadia R conference 2024

Examples of ML



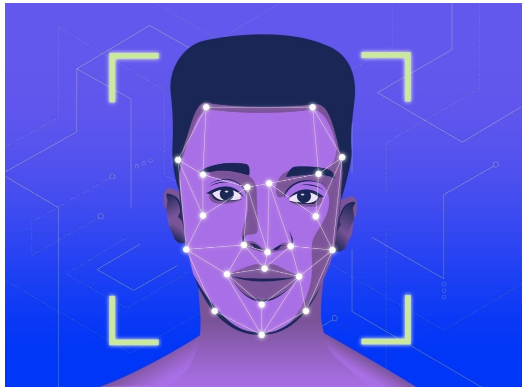


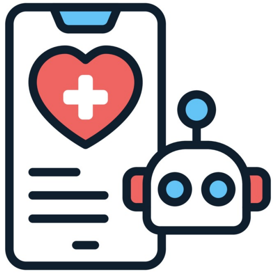
Stock images

When is ML used?

- High-dimensional data

  More features/variables than rows increases complexity of data.





Stock images

When is ML used?

- High-dimensional data

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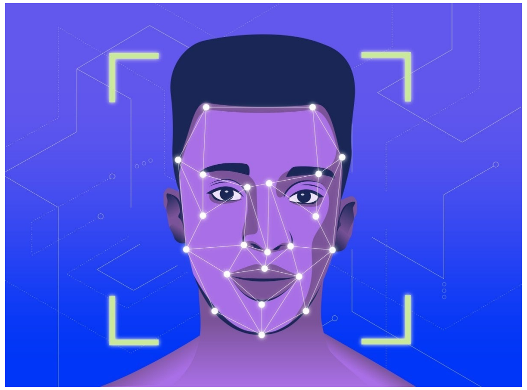
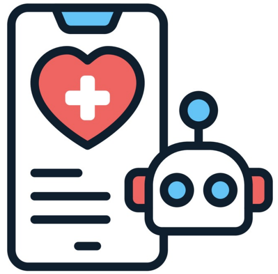
- Non-linear relationships

  Indirect relationship between predictors and outcome.





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When is ML used?

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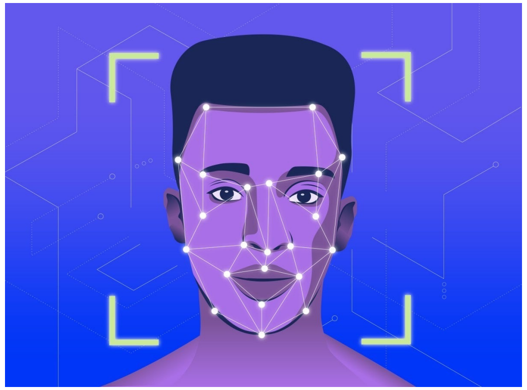
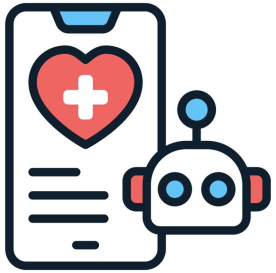
- Unstructured data

  Non-tabular data like text, images, audio.





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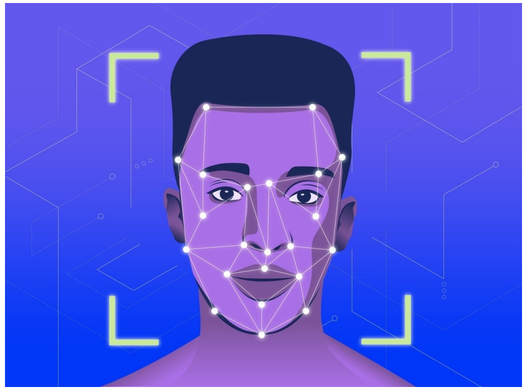
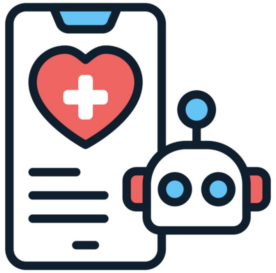
- Scalability

  Ability to handle millions or billions of data points.





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Disclaimer!

This talk will not cover:

- R vs python for ML
- How to choose ML methods
- Pros and cons of using R for ML

Building an ML project

Processing data

Picking and training your ML model

Testing the performance of ML models

Redbubble, Adobe stock

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Data processing

- Exploratory data analysis
- Handle missing data
- Outliers
- Feature engineering
- Feature scaling
- Splitting data into training and validation sets

```
# Example
library(dplyr)
library(ggplot2)

# Summary statistics
summary(mtcars)

# Visualization
ggplot(mtcars, aes(x=mpg, y=hp)) + geom_point()
```

Data processing

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mice

stekhoven/
missForest

missForest is a nonparametric, mixed-type imputation method for basically any type of data for the statistical software R.

3 Contributors | 11 Issues | 87 Stars | 23 Forks

```r
# Example
library(mice)
library(missForest)

# Remove rows with missing values
clean_data <- na.omit(mtcars)

# Multiple imputation
imputed_data <- mice(mtcars, m=5, maxit=50, method='pmm', seed=500)

# Imputation using Random Forests
imputed_data_rf <- missForest(mtcars)
```

Packages for imputation in R: https://www.analyticsvidhya.com/blog/2016/03/tutorial-powerful-packages-imputing-missing-values/

Data processing

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```r
# Example
library(dplyr)
library(ggplot2)

# Identify outliers using boxplot
boxplot(mtcars$mpg)

# Remove outliers
clean_data <- mtcars %>% filter(mpg < quantile(mpg, 0.95))
```

Data processing

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caret

dplyr

```r
# Example
library(dplyr)
library(caret)

# Create new variable
mtcars <- mtcars %>% mutate(power_to_weight = hp / wt)

# Create dummy variables
dummies <- dummyVars(~., data=mtcars)
mtcars_dummies <- predict(dummies, newdata=mtcars)
```

Data processing

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```r
# Example
library(caret)
library(scales)

# Standardize variables
scaled_data <- scale(mtcars)

# Pre-process using caret
preProc <- preProcess(mtcars, method=c("center", "scale"))
mtcars_scaled <- predict(preProc, mtcars)
```

Data processing

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caret

cran/**caTools**

❗ This is a read-only mirror of the CRAN R package repository. caTools — Tools: Moving Window Statistics, GIF, Base64,...

META CRAN

2 Contributors · 0 Issues · 7 Stars · 3 Forks

```r
# Example
library(caret)
library(caTools)

# Using caret
set.seed(123)
trainIndex <- createDataPartition(mtcars$mpg, p=0.7, list=FALSE)
train_data <- mtcars[trainIndex,]
test_data <- mtcars[-trainIndex,]

# Using caTools
set.seed(123)
split <- sample.split(mtcars$mpg, SplitRatio=0.7)
train_data <- subset(mtcars, split==TRUE)
test_data <- subset(mtcars, split==FALSE)
```

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Redbubble, Adobe stock

Types of ML algorithms

Supervised learning

- algorithm is trained on a labeled dataset
- each input is paired with the correct output

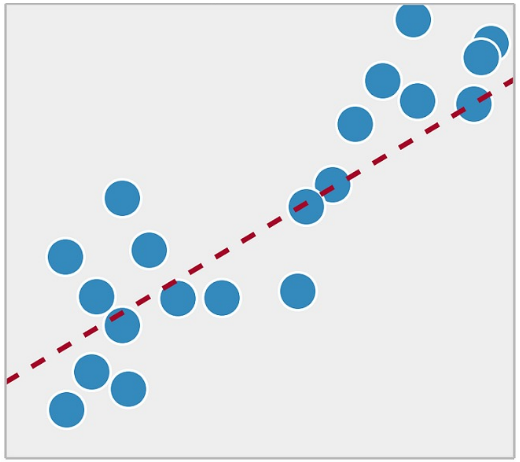
Unsupervised learning

- algorithm works with unlabeled data
- finds patterns or structures
- no explicit guidance

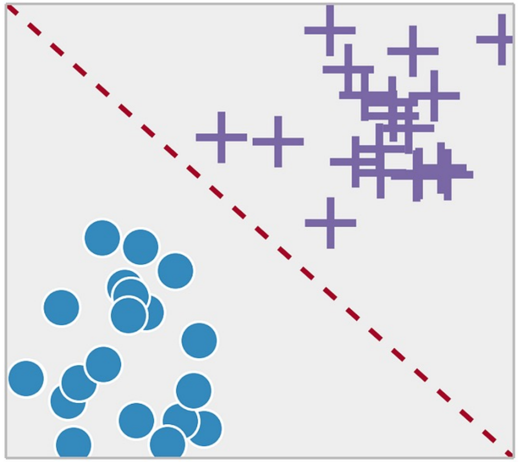
Types of ML algorithms

Supervised learning

Regression

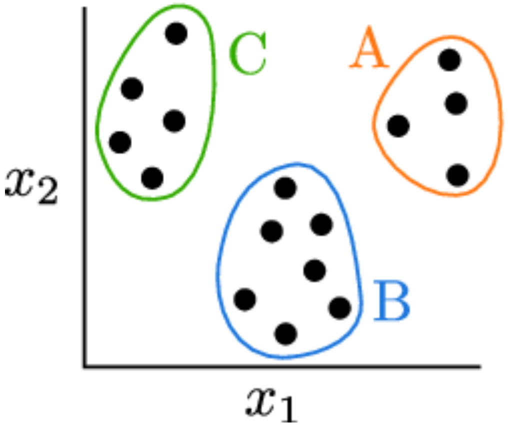


Classification

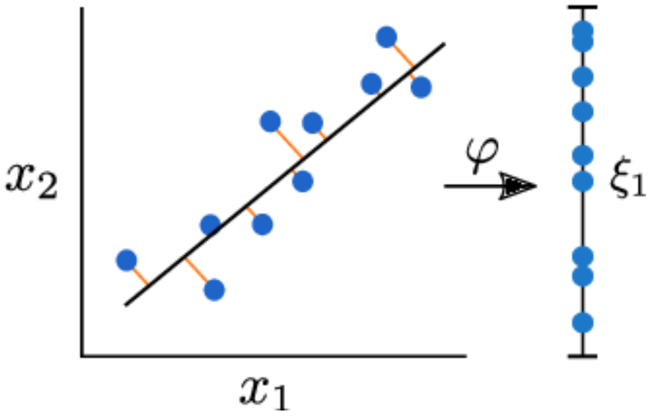


Unsupervised learning

Clustering

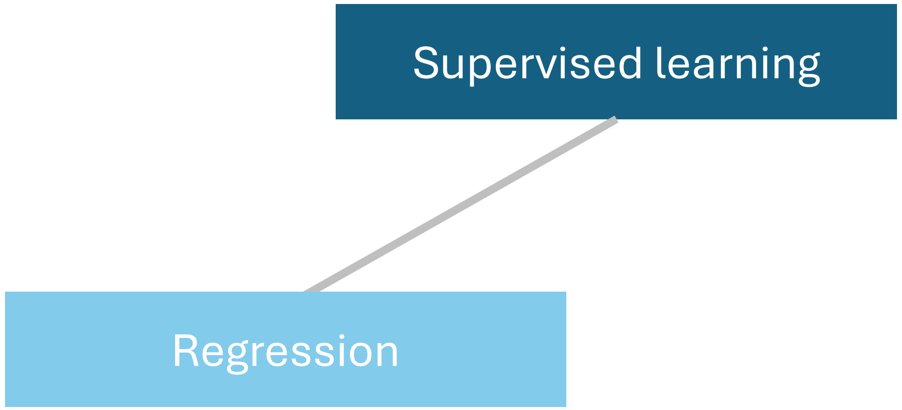


Dimensionality reduction



https://towardsdatascience.com/supervised-vs-unsupervised-learning-14f68e32ea8d
https://www.researchgate.net/publication/344783581_A_Perspective_on_Machine_Learning_Methods_in_Turbulence_Modelling

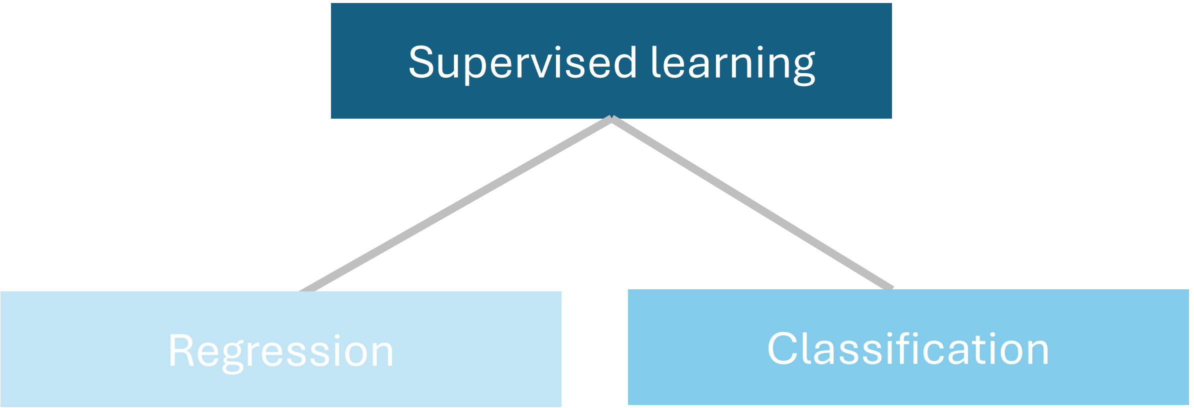
Supervised learning



- **glmnet**: For regularized generalized linear models (lasso, ridge, elastic net)
- **randomForest** or **ranger**: For random forest regression
- **xgboost**: For gradient boosting regression
- **rpart**: For decision tree regression
- **kernlab**: For support vector regression

```
#glmnet: For regularized generalized linear models (lasso, ridge, elastic net)
# Example data
x <- matrix(rnorm(100*20), 100, 20)
y <- rnorm(100)

# Fit a lasso model
fit <- glmnet(x, y, alpha = 1)

#randomForest: For random forest regression
# Example data
data(iris)
set.seed(42)

# Fit a random forest model
fit <- randomForest(Sepal.Length ~ ., data = iris)

#xgboost: For gradient boosting regression
# Example data
data(iris)
set.seed(42)
train <- as.matrix(iris[, -1])
label <- iris$Sepal.Length

# Fit a gradient boosting model
fit <- xgboost(data = train, label = label, nrounds = 100, objective = "reg:squared

#rpart: For decision tree regression
# Example data
data(iris)

# Fit a decision tree model
fit <- rpart(Sepal.Length ~ ., data = iris)

#kernlab: For support vector regression
# Example data
data(iris)

# Fit a support vector regression model
fit <- ksvm(Sepal.Length ~ ., data = iris, type = "eps-svr")
```

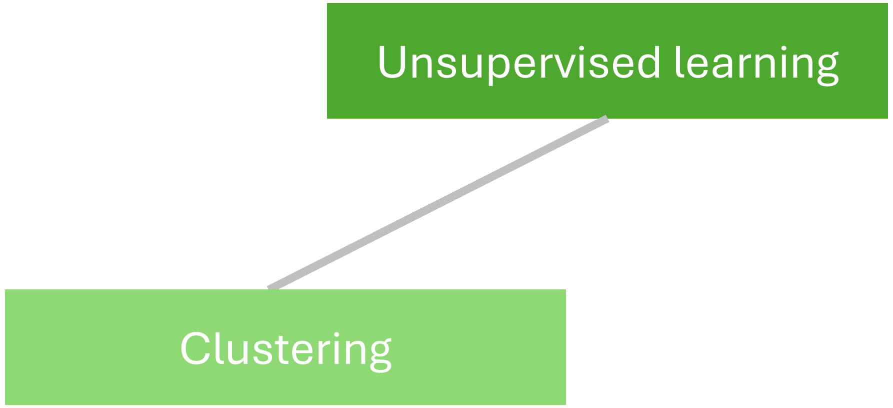
Supervised learning



- **caret:** For various classification algorithms and model training
- **randomForest**: For random forest classification
- **xgboost:** For gradient boosting classification
- **e1071:** For support vector machines and naive Bayes
- **rpart:** For decision tree classification
- **glmnet**: For regularized logistic regression
- **naivebayes:** For naive Bayes classification

```r
#caret: For various classification algorithms and model training
# Example data
data(iris)
set.seed(42)

# Train a model using caret
fit <- train(Species ~ ., data = iris, method = "rf")

#randomForest: For random forest classification
# Example data
data(iris)
set.seed(42)

# Fit a random forest model
fit <- randomForest(Species ~ ., data = iris)

#xgboost: For gradient boosting classification
# Example data
data(iris)
set.seed(42)
train <- as.matrix(iris[, -5])
label <- as.numeric(iris$Species) - 1

# Fit a gradient boosting model
fit <- xgboost(data = train, label = label, nrounds = 100, objective = "multi:softp

#e1071: For support vector machines and naive Bayes
# Example data
data(iris)

# Fit a support vector machine model
fit_svm <- svm(Species ~ ., data = iris)

# Fit a naive Bayes model
fit_nb <- naiveBayes(Species ~ ., data = iris)

#rpart: For decision tree classification
# Example data
data(iris)

# Fit a decision tree model
fit <- rpart(Species ~ ., data = iris)
```

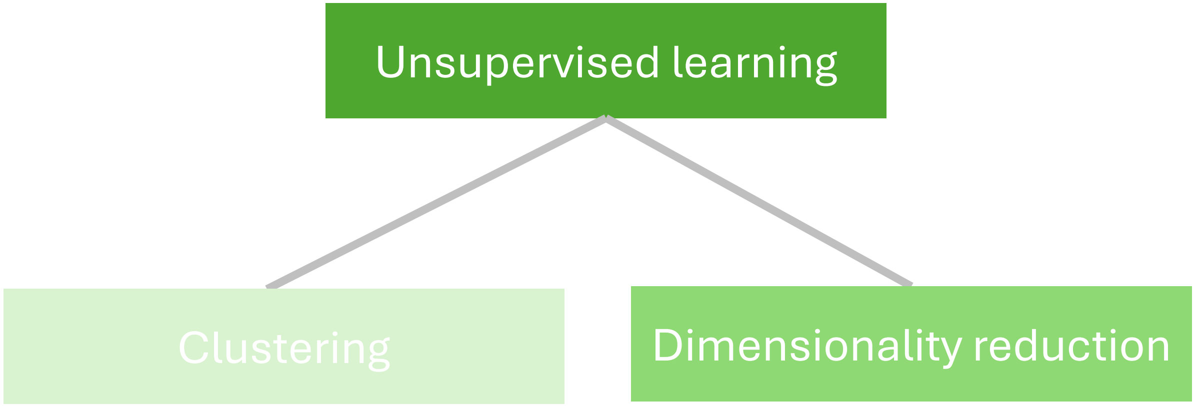
Unsupervised learning



- **stats:** For k-means clustering (built-in R package)
- **cluster:** For various clustering algorithms including hierarchical clustering
- **dbscan:** For density-based clustering

```r
#stats: For k-means clustering (built-in R package)
# Example data
data(iris)

# Perform k-means clustering
fit <- kmeans(iris[, -5], centers = 3)

#cluster: For various clustering algorithms including hierarchical clustering
# Install and load the package
install.packages("cluster")
library(cluster)

# Example data
data(iris)

# Perform hierarchical clustering
fit <- agnes(iris[, -5])

#dbscan: For density-based clustering
# Install and load the package
install.packages("dbscan")
library(dbscan)

# Example data
data(iris)

# Perform DBSCAN clustering
fit <- dbscan(iris[, -5], eps = 0.5, minPts = 5)
```

Unsupervised learning



- **stats**: For principal component analysis (PCA) (built-in R package)
- **FactoMineR:** For various dimensionality reduction techniques
- **Rtsne:** For t-SNE (t-Distributed Stochastic Neighbor Embedding)

```r
#stats: For principal component analysis (PCA) (built-in R package)
# Example data
data(iris)

# Perform PCA
fit <- prcomp(iris[, -5], scale. = TRUE)

#FactoMineR: For various dimensionality reduction techniques
# Install and load the package
install.packages("FactoMineR")
library(FactoMineR)

# Example data
data(iris)

# Perform PCA using FactoMineR
fit <- PCA(iris[, -5], graph = FALSE)

# Rtsne: For t-SNE (t-Distributed Stochastic Neighbor Embedding)
# Install and load the package
install.packages("Rtsne")
library(Rtsne)

# Example data
data(iris)

# Perform t-SNE
fit <- Rtsne(as.matrix(iris[, -5]))
```

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Regression

glmnet
randomForest or **ranger**
xgboost
rpart
kernlab

Classification

caret
randomForest
xgboost
e1071
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glmnet
naivebayes

Unsupervised learning

Clustering

stats
cluster
dbscan

Dimensionality reduction

stats or **PCATools**
FactoMineR
Rtsne

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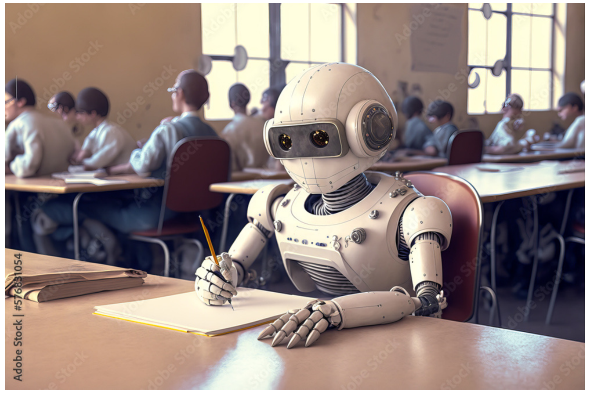

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Testing ML models

- **Classification Metrics**
  - Accuracy using **caret**
  - Precision and Recall using **caret**
  - F1 Score using **caret**
  - AUC-ROC using **pROC** or **ROCit**
- **Regression Metrics**
  - RMSE (Root Mean Squared Error)
  - R-squared (R^2)
- **Visualization Techniques**
  - ROC Curves
  - Density Plots and Boxplots

```r
# Load necessary libraries
library(caret)
library(pROC)

# Load dataset
data(mtcars)

# Split data into training and testing sets
set.seed(123)
trainIndex <- createDataPartition(mtcars$mpg, p = .8,
                                  list = FALSE,
                                  times = 1)
trainData <- mtcars[ trainIndex,]
testData  <- mtcars[-trainIndex,]

# Make predictions
predictions_prob <- predict(model, testData, type = "response")
predictions <- ifelse(predictions_prob > 0.5, 1, 0)
predictions <- as.factor(predictions)

# Create a confusion matrix
conf_matrix <- confusionMatrix(predictions, testData$Species, positive = "1")
print(conf_matrix)

# Extract metrics
accuracy <- conf_matrix$overall['Accuracy']
precision <- conf_matrix$byClass['Pos Pred Value']
recall <- conf_matrix$byClass['Sensitivity']
f1_score <- 2 * (precision * recall) / (precision + recall)

# ROC Curve
roc_obj <- roc(testData$Species, predictions_prob)
plot(roc_obj)
```

Conclusion

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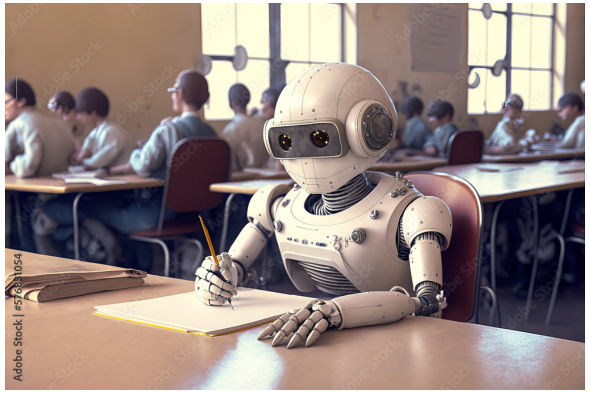

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Thank you