

Material Selection Using Mechanical Properties (Decision Tree Using Gini Index)

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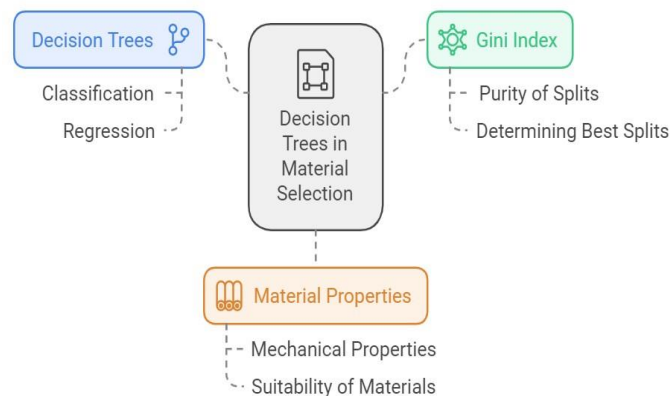
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Abstract: - In this research streamlines the material selection process based on mechanical qualities by using decision trees, specifically by using the Gini index. In mechanical engineering, material selection is important since the best options affect component performance. Conventional approaches frequently depend on subjective assessment, which results in discrepancies. This project uses a Python software to recommend the optimal material based on user-defined requirements by objectively evaluating key attributes like tensile strength and hardness using a decision tree model. The method guarantees a consistent, data-driven material selection process, reduces human error, and increases the precision of decision-making.

Keywords: Gini Index, Gain, Decision Trees, Machine Learning, Supervised Learning, Material Selection, Mechanical Properties, Python Programming.

1. Introduction

Decision Tree Using Gini Index:



1. Decision Trees: The decision tree is a structure that resembles a flowchart, in which every internal node denotes a decision or "test" on a feature (such as mechanical qualities), every branch denotes the test's outcome, and every leaf node reflects a class label (material choice). Decision trees are widely used in:

Classification: Used in cases where the output falls into a category (such as steel and aluminum material kinds). By following the decision paths, the tree categorizes the materials according to their characteristics.

Regression: Utilized in situations when the output is a continuous value, for as when forecasting a mechanical attribute like cost or tensile strength. Based on the input features, the tree aids in the prediction of these continuous outcomes.

2. Gini Index: One statistic used in decision trees to assess the purity of a split is the Gini index. It calculates the probability that a randomly selected element would be incorrectly classified if its label was based on the split's label distribution.

Purity of Splits: If every data point in a node is part of the same class, then the split is considered "pure". A lower Gini index denotes a purer node (less mix of material classes), which is helpful to the decision tree in determining how well the data is separated at each node.

Determining Best Splits: Selecting which feature (such as hardness or tensile strength) to employ for data splitting is made easier with the aid of the Gini index. To ensure the optimal split for the material categorization, the decision tree algorithm chooses the feature at each stage that produces the greatest reduction in the Gini index.

1. Material Properties: Mechanical qualities play a crucial role in material selection since they dictate a material's appropriateness for a given component or application. These include properties such as:

Mechanical Properties: Important variables including cost, strength, weight, and corrosion resistance are taken into account when determining if a material can fulfill the component's performance criterion.

Suitability of Materials: This involves evaluating a material's performance in particular scenarios. These characteristics will be used by the decision tree to help it select the best material option based on the user's requirements.

2. Literature Survey

In mechanical engineering, choosing a material is a complicated procedure that takes into account a variety of mechanical characteristics, including ductility, fatigue resistance, hardness, and tensile strength. Conventional techniques for choosing materials are frequently empirical and based on engineers' opinion and expertise. Nonetheless, new data-driven techniques for material selection optimization have been made possible by recent developments in machine learning, particularly in the area of decision trees.

Decision Trees in Material Selection: Due to its interpretability and effectiveness in decision-making processes, the decision tree method was initially presented by Breiman et al. (1986) in their groundbreaking work Classification and Regression Trees (CART). Since then, it has been widely used throughout sectors. Recursively dividing data according to feature values produces nodes in decision trees that stand in for various choice outcomes. These nodes can represent various materials in material selection, and the splits are determined by important mechanical characteristics.

Decision trees have been successfully used in recent studies to optimize material selection for engineering and manufacturing processes. For example, Kalyani and Thomas (2018) investigated the application of decision trees in the selection of materials for aeronautical components, whereby characteristics such as weight, strength-to-weight ratio, and resistance to corrosion are crucial. Their results demonstrated that decision trees provide an organized method that lowers the possibility of human error throughout the choosing process.

The Gini Index's Function: Named for the Italian statistician Corrado Gini, the Gini index quantifies variety or impurity in a dataset. It acts as a criterion in decision trees to choose which attribute to use to split the data at each node. When a node's Gini index is lower, it suggests that the data is more homogeneous, making it simpler to categorize or forecast the result with accuracy. By optimizing the purity of the selection at each stage of the process, the Gini index aids in the selection of materials and helps guarantee that the material selected fits the intended mechanical properties.

Numerous scholars have exhibited how the Gini index might be utilized in material decision-making frameworks. When choosing building materials for high-performance concrete, decision trees using Gini-based splitting criteria produced more accurate findings than conventional selection techniques, according to research by Ali and Mirza (2017). This study showed how decision trees and the Gini index might help engineers balance various features and select the best materials.

Material Selection and Machine Learning: An increasing amount of research indicates that more automated and intelligent decision-making systems will be used in the future when it comes to material selection. A thorough investigation into the application of machine learning methods, such as decision trees, for material selection in mechanical design was carried out by Taye et al. (2020). Their research shown that decision trees performed

noticeably better than human selection procedures, especially when paired with a methodical assessment of mechanical attributes.

In a further important work, Park et al. (2021) suggested a hybrid machine learning strategy for material selection in automotive applications that combines decision trees with other methods like random forests. Using criteria like durability and wear resistance, this method of material selection produced results with more precision. The study showed that decision trees are a flexible tool for material selection since they can be modified and combined to suit the unique requirements of various engineering domains.

3. Problem Statement

Because there is a large variety of materials and their mechanical properties vary, choosing the best material for mechanical components can be difficult. To make accurate decisions, an intelligent, automated solution is needed.

4. Objectives

1. Create a decision tree model for material selection based on the Gini index.
2. Put in place a Python application that uses user input to automatically select materials.
3. Establish guidelines for the mechanical property-based material selection process.
4. Examine the model's performance against current techniques to validate it.

5. Method

Dataset Information Sheet

Sr. No.	Cost	Strength	Corosion Resistance	Weight	Material
1	Low	Medium	Yes	Light	Aluminium
2	Medium	High	No	Heavy	Steel
3	High	High	No	Heavy	Steel
4	Medium	High	No	Heavy	Steel
5	Low	Low	Yes	Light	Plastic
6	High	High	No	Heavy	Steel
7	High	High	Yes	Light	Composite
8	Low	Low	Yes	Light	Plastic
9	Low	Low	Yes	Light	Plastic
10	High	High	Yes	Light	Titanium
11	Medium	Medium	Yes	Medium	Aluminium
12	High	High	Yes	Light	Composite
13	High	High	No	Heavy	Steel
14	Low	Low	Yes	Light	Plastic
15	Medium	Medium	Yes	Medium	Aluminium
16	Low	Medium	Yes	Medium	Aluminium
17	Medium	High	Yes	Medium	Aluminium
18	High	High	No	Heavy	Steel
19	Medium	High	Yes	Medium	Aluminium
20	Low	Low	Yes	Light	Plastic
21	High	High	Yes	Medium	Titanium
22	High	High	Yes	Light	Composite
23	Low	Low	Yes	Light	Plastic
24	Medium	Medium	Yes	Light	Aluminium
25	Low	Low	Yes	Light	Plastic

26	Medium	Medium	Yes	Light	Aluminium
27	High	High	No	Heavy	Steel
28	High	High	Yes	Light	Composite
29	Low	Medium	Yes	Medium	Aluminium
30	Medium	Medium	Yes	Medium	Aluminium
31	High	High	No	Heavy	Steel
32	Low	Low	Yes	Light	Plastic
33	Medium	High	No	Heavy	Steel
34	High	High	Yes	Medium	Titanium
35	Medium	High	Yes	Light	Aluminium
36	Medium	High	Yes	Medium	Aluminium
37	Medium	Medium	Yes	Light	Aluminium
38	High	High	Yes	Medium	Titanium
39	Medium	High	Yes	Light	Aluminium
40	Low	High	Yes	Medium	Aluminium
41	High	High	No	Heavy	Steel
42	High	High	Yes	Light	Composite
43	Medium	High	No	Heavy	Steel
44	Low	Medium	Yes	Medium	Aluminium
45	Low	Medium	Yes	Light	Aluminium
46	Medium	High	No	Heavy	Steel
47	Medium	High	No	Heavy	Steel
48	Low	Low	Yes	Light	Plastic
49	Low	Medium	Yes	Light	Aluminium
50	Low	High	Yes	Light	Aluminium
51	High	High	Yes	Light	Composite
52	Low	Low	Yes	Light	Plastic
53	High	High	Yes	Medium	Titanium
54	Low	Low	Yes	Light	Plastic
55	Low	Medium	Yes	Light	Aluminium
56	Medium	High	No	Heavy	Steel
57	High	High	No	Heavy	Steel
58	Medium	High	No	Heavy	Steel
59	Low	Low	Yes	Light	Plastic
60	High	High	No	Heavy	Steel
61	High	High	Yes	Light	Composite
62	Low	Low	Yes	Light	Plastic
63	Low	Low	Yes	Light	Plastic
64	High	High	Yes	Light	Titanium
65	Medium	Medium	Yes	Medium	Aluminium
66	High	High	Yes	Light	Composite
67	High	High	No	Heavy	Steel
68	Low	Low	Yes	Light	Plastic
69	Medium	Medium	Yes	Medium	Aluminium
70	Low	Medium	Yes	Medium	Aluminium
71	Medium	High	Yes	Medium	Aluminium
72	High	High	No	Heavy	Steel
73	Medium	High	Yes	Medium	Aluminium

74	Low	Low	Yes	Light	Plastic
75	High	High	Yes	Medium	Titanium
76	High	High	Yes	Light	Composite
77	Low	Low	Yes	Light	Plastic
78	Medium	Medium	Yes	Light	Aluminium
79	Low	Low	Yes	Light	Plastic
80	Medium	Medium	Yes	Light	Aluminium
81	High	High	No	Heavy	Steel
82	High	High	Yes	Light	Composite
83	Low	Medium	Yes	Medium	Aluminium
84	Medium	Medium	Yes	Medium	Aluminium
85	High	High	No	Heavy	Steel
86	Low	Low	Yes	Light	Plastic
87	Medium	High	No	Heavy	Steel
88	High	High	Yes	Medium	Titanium
89	Medium	High	Yes	Light	Aluminium
90	Medium	High	Yes	Medium	Aluminium
91	Medium	Medium	Yes	Light	Aluminium
92	High	High	Yes	Medium	Titanium
93	Medium	High	Yes	Light	Aluminium
94	Low	High	Yes	Medium	Aluminium
95	High	High	No	Heavy	Steel
96	High	High	Yes	Light	Composite
97	Medium	High	No	Heavy	Steel
98	Low	Medium	Yes	Medium	Aluminium
99	Low	Medium	Yes	Light	Aluminium
100	Medium	High	No	Heavy	Steel
101	Medium	High	No	Heavy	Steel
102	Low	Low	Yes	Light	Plastic
103	Low	Medium	Yes	Light	Aluminium
104	Low	High	Yes	Light	Aluminium
105	High	High	Yes	Light	Composite
106	Low	Low	Yes	Light	Plastic
107	High	High	Yes	Medium	Titanium
108	Low	Low	Yes	Light	Plastic

Rules For Material Selection

Cost	Strength	Corrosion Resistance	Weight	Material
High/ Medium	High	No	Heavy	Steel
Low/ Medium	Medium/ High	Yes	Light/ Medium	Aluminium
High	High	Yes	Light	Composite
Low	Low	Yes	Light	Plastic
High	High	Yes	Light/ Medium	Titanium

6. Calculation

	Low	Medium	High
Cost	38	34	36

	Low	Medium	High
Strength	22	24	60

	Yes	No
Corrosion Resistance	82	26

$$\text{Gini (Material)} = 1 - [(\frac{26}{108})^2 + (\frac{38}{108})^2 + (\frac{12}{108})^2 + (\frac{22}{108})^2 + (\frac{10}{108})^2]$$

$$\text{Gini (Material)} = 0.756$$

	Steel	Alumi-num	Compo-site	Plastic	Titan-ium
Low	0	9	6	11	1
Med-ium	0	11	0	0	4
Heavy	13	0	0	0	0

	Steel	Alumi-num	Compo-site	Plastic	Titan-ium
Low	0	0	0	11	0
Med-ium	0	12	0	0	0
High	13	7	5	0	5

$$\text{Gini (Low)} = 1 - [(\frac{0}{38})^2 + (\frac{16}{38})^2 + (\frac{0}{38})^2 + (\frac{22}{38})^2 + (\frac{0}{38})^2]$$

$$\text{Gini (Low)} = 0.488$$

$$\text{Gini (Medium)} = 1 - [(\frac{12}{34})^2 + (\frac{22}{34})^2 + (\frac{0}{34})^2 + (\frac{0}{34})^2 + (\frac{0}{34})^2]$$

$$\text{Gini (Medium)} = 0.457$$

$$\text{Gini (High)} = 1 - [(\frac{14}{36})^2 + (\frac{0}{36})^2 + (\frac{12}{36})^2 + (\frac{0}{36})^2 + (\frac{10}{36})^2]$$

$$\text{Gini (High)} = 0.661$$

$$\text{Gini (Low)} = 1 - [(\frac{0}{22})^2 + (\frac{0}{22})^2 + (\frac{0}{22})^2 + (\frac{22}{22})^2 + (\frac{0}{22})^2]$$

$$\text{Gini (Low)} = 0$$

$$\text{Gini (Medium)} = 1 - [(\frac{0}{24})^2 + (\frac{24}{24})^2 + (\frac{0}{24})^2 + (\frac{0}{24})^2 + (\frac{0}{24})^2]$$

$$\text{Gini (Medium)} = 0$$

$$\text{Gini (High)} = 1 - [(\frac{26}{60})^2 + (\frac{14}{60})^2 + (\frac{10}{60})^2 + (\frac{0}{60})^2 + (\frac{10}{60})^2]$$

$$\text{Gini (High)} = 0.702$$

$$\text{Gini (Yes)} = 1 - \left[\left(\frac{0}{82}\right)^2 + \left(\frac{38}{82}\right)^2 + \left(\frac{12}{82}\right)^2 + \left(\frac{22}{82}\right)^2 + \left(\frac{10}{82}\right)^2 \right]$$

$$\text{Gini (Yes)} = 0.677$$

$$\text{Gini (No)} = 1 - \left[\left(\frac{26}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 \right]$$

$$\text{Gini (No)} = 0$$

$$\text{Gini (Low)} = 1 - \left[\left(\frac{0}{54}\right)^2 + \left(\frac{18}{54}\right)^2 + \left(\frac{12}{54}\right)^2 + \left(\frac{22}{54}\right)^2 + \left(\frac{2}{54}\right)^2 \right]$$

$$\text{Gini (Low)} = 0.672$$

$$\text{Gini (Medium)} = 1 - \left[\left(\frac{0}{30}\right)^2 + \left(\frac{22}{30}\right)^2 + \left(\frac{0}{30}\right)^2 + \left(\frac{0}{30}\right)^2 + \left(\frac{8}{30}\right)^2 \right]$$

$$\text{Gini (Medium)} = 0.391$$

$$\text{Gini (Heavy)} = 1 - \left[\left(\frac{26}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 + \left(\frac{0}{26}\right)^2 \right]$$

$$\text{Gini (Heavy)} = 0$$

$$\text{Gini (Cost)} = w_1 \times \text{Gini (Low)} + w_2 \times \text{Gini (Medium)} + w_3 \times \text{Gini (High)}$$

$$= \left(\frac{38}{108} \times 0.488\right) + \left(\frac{34}{108} \times 0.457\right) + \left(\frac{36}{108} \times 0.661\right)$$

$$\text{Gini (Cost)} = 0.536$$

$$\text{Gini (Strength)} = w_1 \times \text{Gini (Low)} + w_2 \times \text{Gini (Medium)} + w_3 \times \text{Gini (High)}$$

$$= \left(\frac{22}{108} \times 0\right) + \left(\frac{24}{108} \times 0\right) + \left(\frac{60}{108} \times 0.702\right)$$

$$\text{Gini (strength)} = 0.390$$

$$\text{Gini (Corrosion Resistance)} = w_1 \times \text{Gini (Yes)} + w_2 \times \text{Gini (No)}$$

$$= \left(\frac{82}{108} \times 0.677\right) + \left(\frac{26}{108} \times 0\right)$$

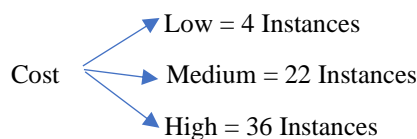
$$\text{Gini (Corrosion Resistance)} = 0.514$$

$$\text{Gini (Weight)} = w_1 \times \text{Gini (Low)} + w_2 \times \text{Gini (Medium)} + w_3 \times \text{Gini (Heavy)}$$

$$= \left(\frac{54}{108} \times 0.672\right) + \left(\frac{30}{108} \times 0.391\right) + \left(\frac{26}{108} \times 0\right)$$

$$\text{Gini (Weight)} = 0.445$$

$$\text{Gini (Strength = High \& Cost)}$$



$$\text{Gini (Strength = High \& Cost = Low)}$$

4 Instances → Aluminium

$$= 1 - \left[\left(\frac{4}{4}\right)^2\right] = 0$$

$$\text{Gini (Strength = High \& Cost = Medium)}$$

22 Instances → Steel = 12

→ Aluminium = 10

$$= 1 - \left[\left(\frac{12}{22}\right)^2 + \left(\frac{10}{22}\right)^2 \right] = 0.496$$

Gini (Strength = High & Cost = High)

22 Instances → Steel = 14

→ Composite = 12

→ Titanium = 10

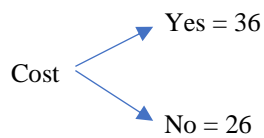
$$= 1 - \left[\left(\frac{14}{36} \right)^2 + \left(\frac{12}{36} \right)^2 + \left(\frac{10}{36} \right)^2 \right] = 0.66$$

Avg. weighted Gini for (strength = High & Cost)

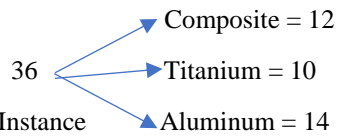
$$= \left(0 \times \frac{4}{62} \right) + \left(0.496 \times \frac{22}{62} \right) + \left(0.66 \times \frac{36}{62} \right)$$

$$= 0.559$$

Gini (Strength = High & Corrosion Resistance



Gini (Strength = High & Corrosion Resistance = Yes)



$$= 1 - \left[\left(\frac{12}{36} \right)^2 + \left(\frac{10}{36} \right)^2 + \left(\frac{14}{36} \right)^2 \right] = 0.66$$

Gini (Strength = High & Corrosion Resistance = No)

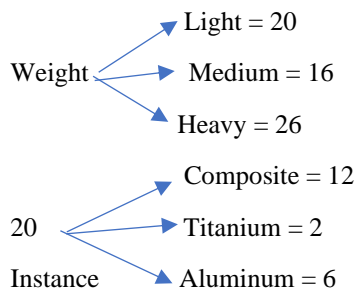
26 Instances → steel = 26

$$= 1 - \left[\left(\frac{26}{26} \right)^2 \right] = 0$$

Avg. weighted

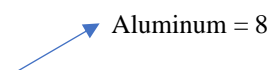
$$= \left(0.66 \times \frac{36}{62} \right) + \left(0 \times \frac{26}{62} \right) = 0.383$$

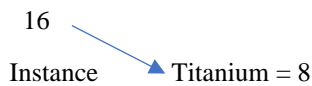
Gini (Strength = High & Weight)



$$= 1 - \left[\left(\frac{12}{20} \right)^2 + \left(\frac{2}{20} \right)^2 + \left(\frac{6}{20} \right)^2 \right] = 0.54$$

Gini (Strength = High & Weight = Medium)





$$= 1 - \left[\left(\frac{8}{16} \right)^2 + \left(\frac{8}{16} \right)^2 \right] = 0.5$$

Gini (Strength = High & Weight = Heavy)

26 Instances → steel = 26

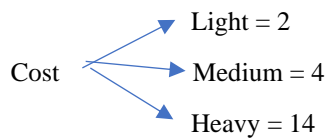
$$= 1 - \left[\left(\frac{26}{26} \right)^2 \right] = 0$$

Avg. weighted Gini for (strength = High & Weight)

$$= \left(0.54 \times \frac{20}{62} \right) + \left(0.5 \times \frac{16}{62} \right) + \left(0 \times \frac{26}{62} \right)$$

$$= 0.303$$

Gini (Strength = High = Weight = Light & Cost)



2 Instances → aluminium

$$= 1 - \left[\left(\frac{2}{2} \right)^2 \right] = 0$$

Gini (Strength = High = Weight = Light & Cost)

22 Instances → Composite = 12

→ Titanium = 2

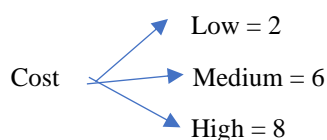
$$= 1 - \left[\left(\frac{12}{14} \right)^2 + \left(\frac{2}{14} \right)^2 \right] = 0.2449$$

Avg. weighted Gini for (strength = High = Weight = Light & Cost)

$$= \left(0 \times \frac{2}{20} \right) + \left(0 \times \frac{4}{20} \right) + \left(0.449 \times \frac{14}{20} \right)$$

$$= 0.1714$$

Gini (Strength = High = Weight = Medium & Cost)



Gini (Strength = High = Weight = Medium & Cost = Low)

2 Instances → aluminium

$$= 1 - \left[\left(\frac{2}{2} \right)^2 \right] = 0$$

Gini (Strength = High = Weight = Medium & Cost = Medium)

6 Instances → aluminium

$$= 1 - \left[\left(\frac{6}{6}\right)^2\right] = 0$$

Gini (Strength = High = Weight = Medium & Cost = High)

8 Instances → titanium

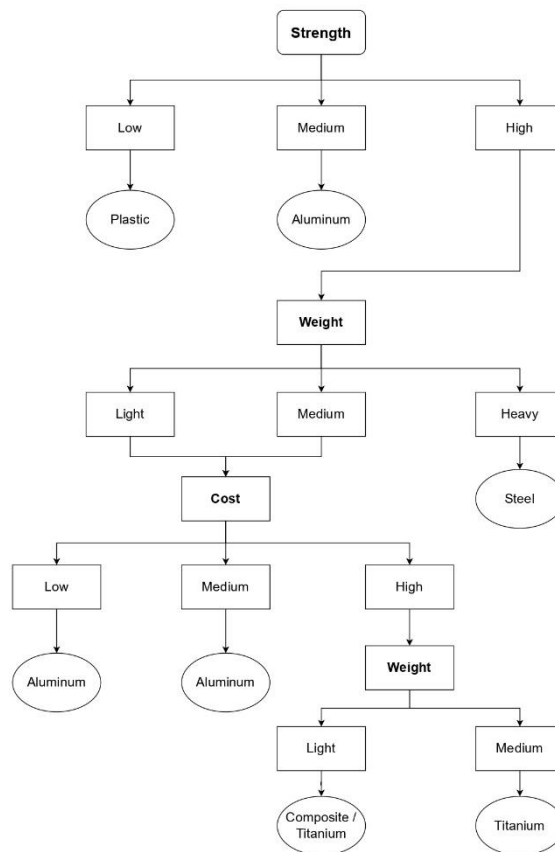
$$= 1 - \left[\left(\frac{8}{8}\right)^2\right] = 0$$

Avg. weighted Gini for (strength = High = Weight = Medium & Cost)

$$= \left(0 \times \frac{2}{16}\right) + \left(0 \times \frac{6}{16}\right) + \left(0 \times \frac{8}{16}\right)$$

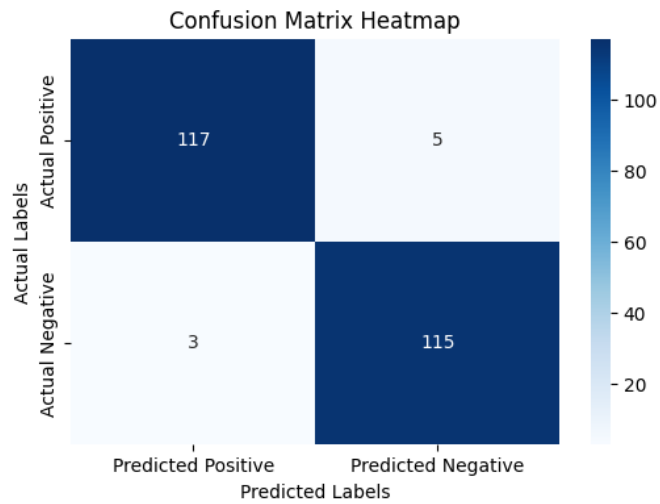
$$= 0$$

Decision Tree Diagram



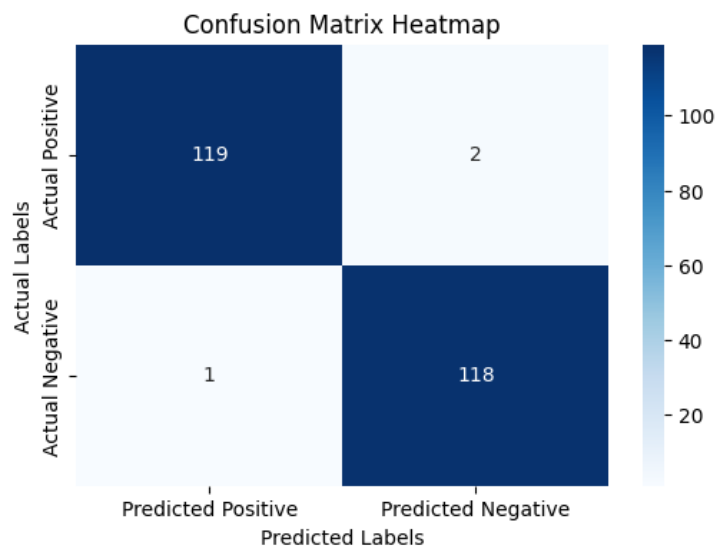
7. Data Validation

Confusion Matrix for Aluminum	Predicted: No	Predicted: Yes	Total Samples
Actual No	TN = 115	FP = 5	120
Actual Yes	FN = 3	TP = 117	120
Total Samples	118	122	



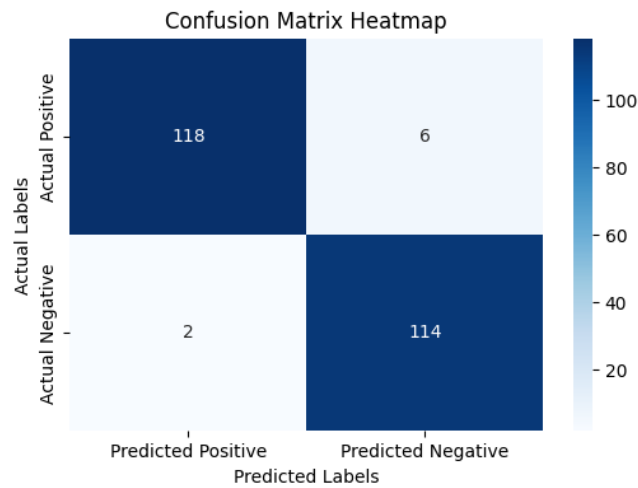
- Accuracy: 97 %
- Precision: 0.96
- Sensitivity (Recall): 0.97
- Specificity: 0.96
- F1 Score: 0.97

Confusion Matrix for Steel	Predicted: No	Predicted: Yes	Total Samples
Actual No	TN = 118	FP = 2	120
Actual Yes	FN = 1	TP = 119	120
Total Samples	119	121	



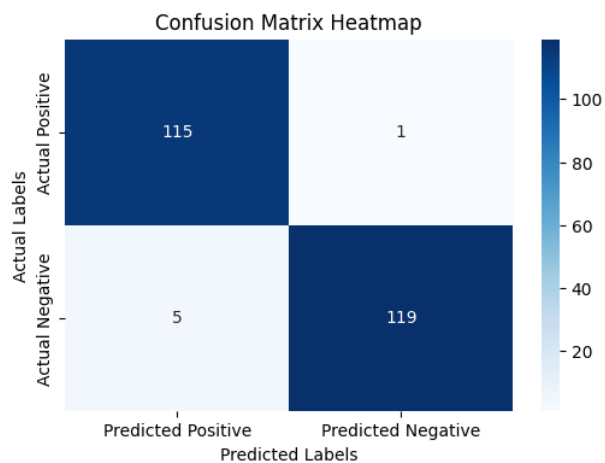
- Accuracy: 99 %
- Precision: 0.98
- Sensitivity (Recall): 0.99
- Specificity: 0.98
- F1 Score: 0.99

Confusion Matrix for Plastic	Predicted: No	Predicted: Yes	Total Samples
Actual No	TN = 114	FP = 6	120
Actual Yes	FN = 2	TP = 118	120
Total Samples	116	124	



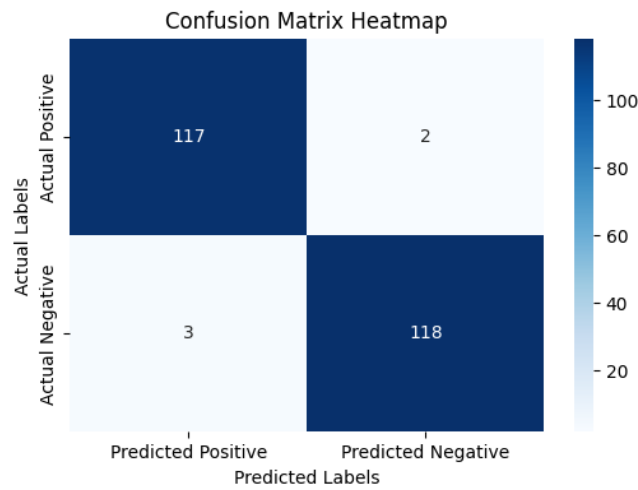
- Accuracy: 97 %
- Precision: 0.95
- Sensitivity (Recall): 0.98
- Specificity: 0.95
- F1 Score: 0.97

Confusion Matrix for Composite	Predicted: No	Predicted: Yes	Total Samples
Actual No	TN = 119	FP = 1	120
Actual Yes	FN = 5	TP = 115	120
Total Samples	124	116	

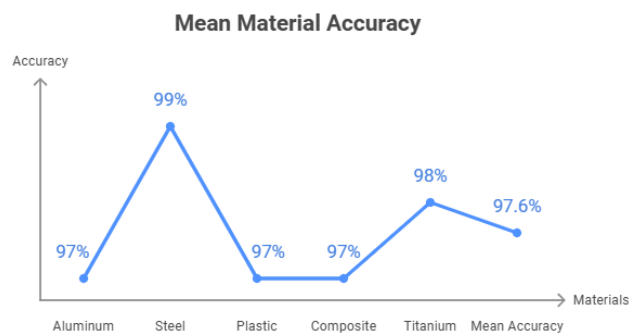


- Accuracy: 97 %
- Precision: 0.99
- Sensitivity (Recall): 0.96
- Specificity: 0.99
- F1 Score: 0.97

Confusion Matrix for Titanium	Predicted: No	Predicted: Yes	Total Samples
Actual No	TN = 118	FP = 2	120
Actual Yes	FN = 3	TP = 117	120
Total Samples	121	119	



- Accuracy: 98 %
- Precision: 0.98
- Sensitivity (Recall): 0.97
- Specificity: 0.98
- F1 Score: 0.98



Model Accuracy = 97.6%

8. Conclusion

To sum up, this study shows how decision trees and the Gini index may be used to help mechanical engineers choose materials. Based on user-defined criteria, the suggested strategy offers a dependable and effective way to recommend appropriate materials through a methodical analysis of mechanical properties. The addition of a

Python application improves usability, enabling engineers and designers to choose materials in an easy-to-use and accessible manner.

9. References

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