Computational Material Design and Discovery of Magnesium Alloys.

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Overview

- Motivation
- Objective
- Background
- Method Implementation
    - Data mining
    - Data preprocessing
    - Building models
- Evaluation and Result Analysis

Motivation

- Engineering alloys are a blend of elements, often a combination of more than 10 deliberate alloying additions. As a consequence, the number of possible alloys that can be produced is (empirically speaking) nearly infinite.

- Magnesium alloys are the lightest engineering materials, and critical to 'light weighting', as they can reduce fuel/energy use, leading to less pollution.

- Today, brake systems, power steering, support brackets and housings are all users of magnesium alloy thanks to its lightweight and strong qualities.
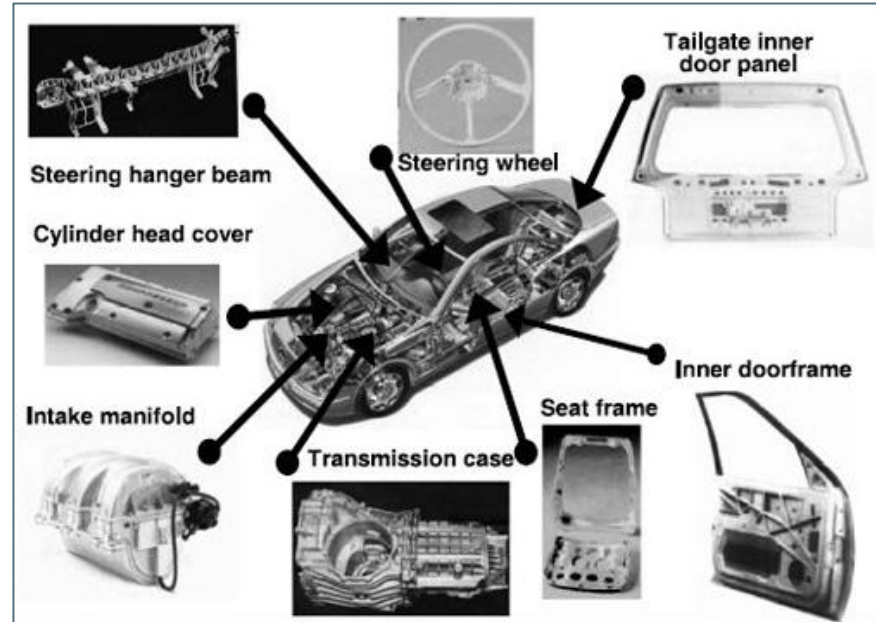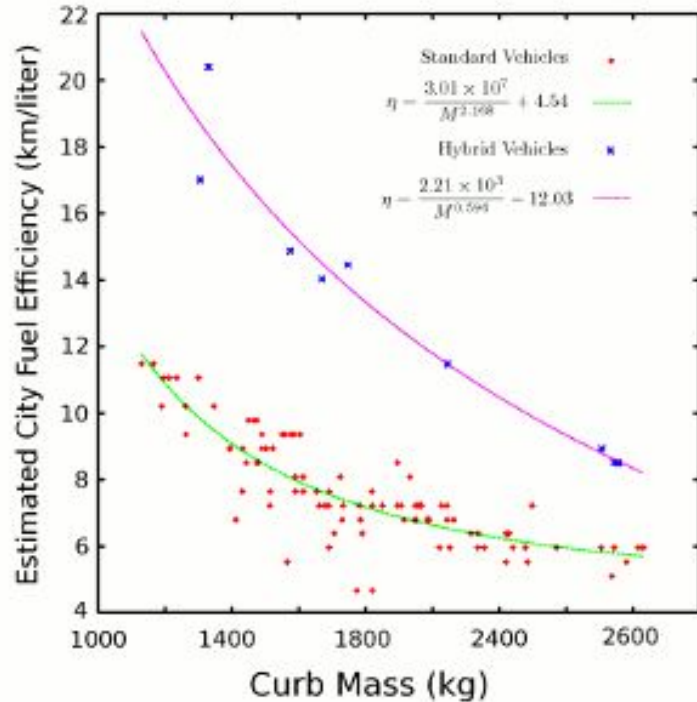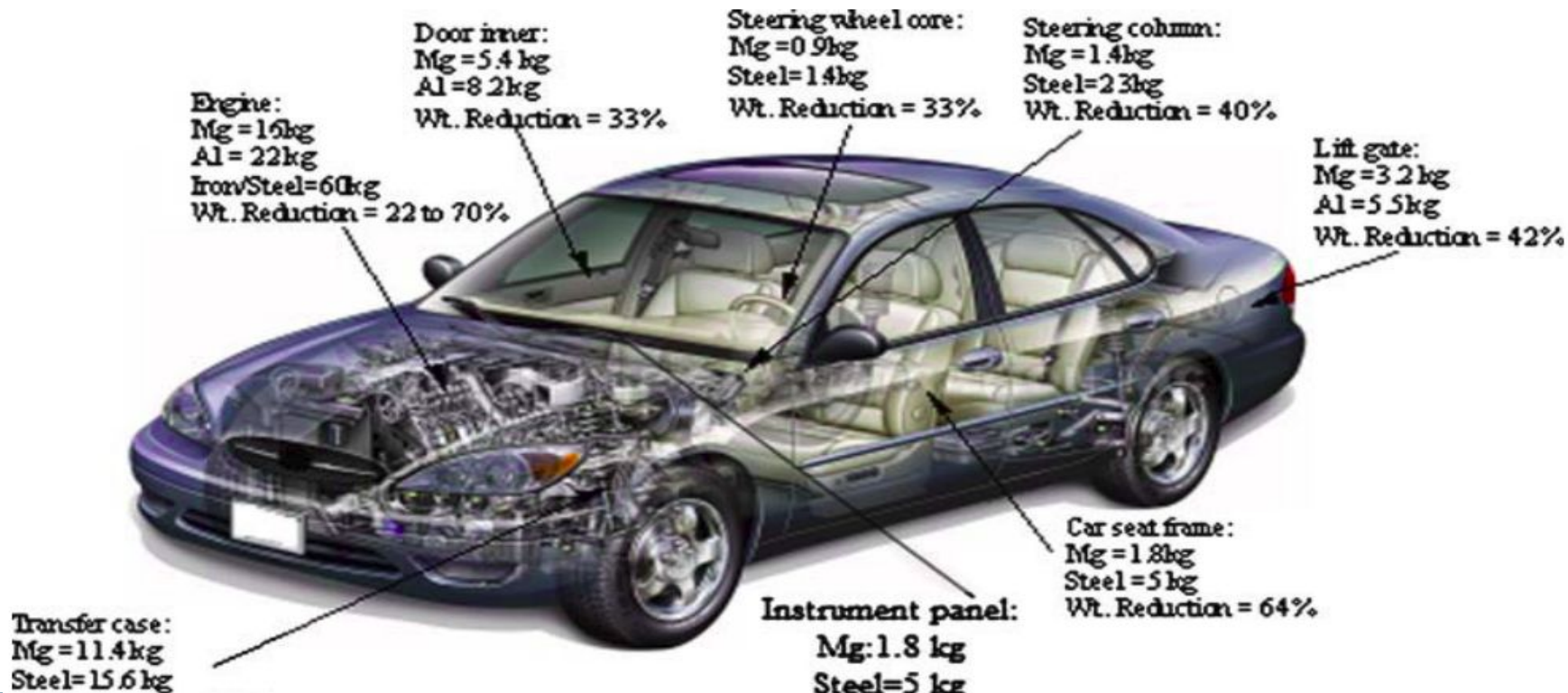

Lightweight chassis

Lightweight roof

Motivation

Magnesium alloys bring down curb mass, dramatically
As Mg weight 4 x less than steel

Motivation

Door inner:
Mg = 5.4 kg
Al = 8.2 kg
Wt. Reduction = 33%

Steering wheel core:
Mg = 0.9kg
Steel=14kg
Wt. Reduction = 33%

Steering column:
Mg = 1.4kg
Steel = 2.3kg
Wt. Reduction = 40%

Engine:
Mg = 16kg
Al = 22kg
Iron/Steel=60kg
Wt. Reduction = 22 to 70%

Lift gate:
Mg = 3.2 kg
Al = 5.5kg
Wt. Reduction = 42%

Transfer case:
Mg = 11.4 kg
Steel = 15.6 kg

Instrument panel:
Mg: 1.8 kg
Steel = 5 kg

Car seat frame:
Mg = 1.8kg
Steel = 5 kg
Wt. Reduction = 64%

Objective

- The Objective of this project is broken into 3 parts.
    - Collect data from various sources
    - Apply machine learning techniques to predict the model's mechanical properties using alloy composition
    - Using the trained model or another technique to find a new optimum composition of Mg.

Background

- Magnesium alloys
- Restrictions of each element in the composition and their maximum solubility.
- Knowledge about the mechanical properties such as Ductlility, Tensile Strength and Yield Strength.
- Use of Machine learning to predict these properties.

Method - Data Mining
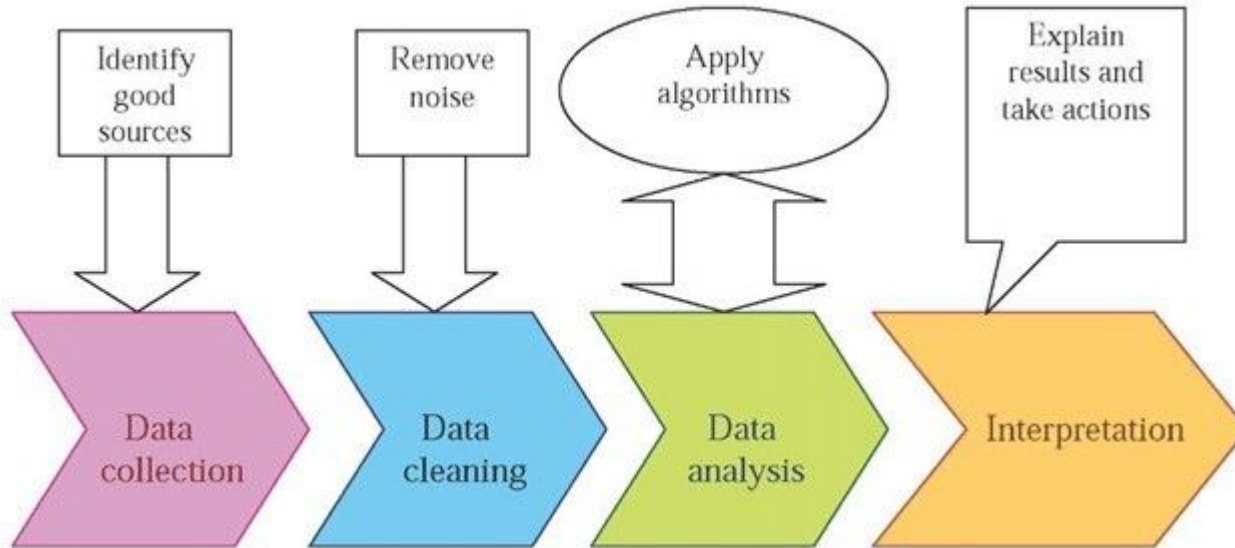
Data Mining

- MATWEB - Professional Material search Web
- CES Material Selection
- Journal Articles
- Research Papers
- Google Scholar

What the data looks like

	Name	Condition	Condition(Numeric)	Mg	Al	Zn	....	Dy	Fe	UTS	YS	Ductility
	Mg-Zn-Ho	Extrusion(230 degree C)	1	93	0	6	....	0	0	280	200	15
	Mg-Zn-Ho	Extrusion(210 degree C)	1	96.9	0	2.7	....	0	0	208	300	20
	AZ61-A2	Extrusion	1	92.23	6.76	0.74	....	0	0	297	319	18
	AZ80-39	Extrusion	1	90.66	8.4	0.6	....	0	0	329	333	13

The processing condition of the alloy (i.e. the "cooking" condition)   +   The composition of the alloy (i.e. the "ingredients" before cooking)   =   The alloy properties

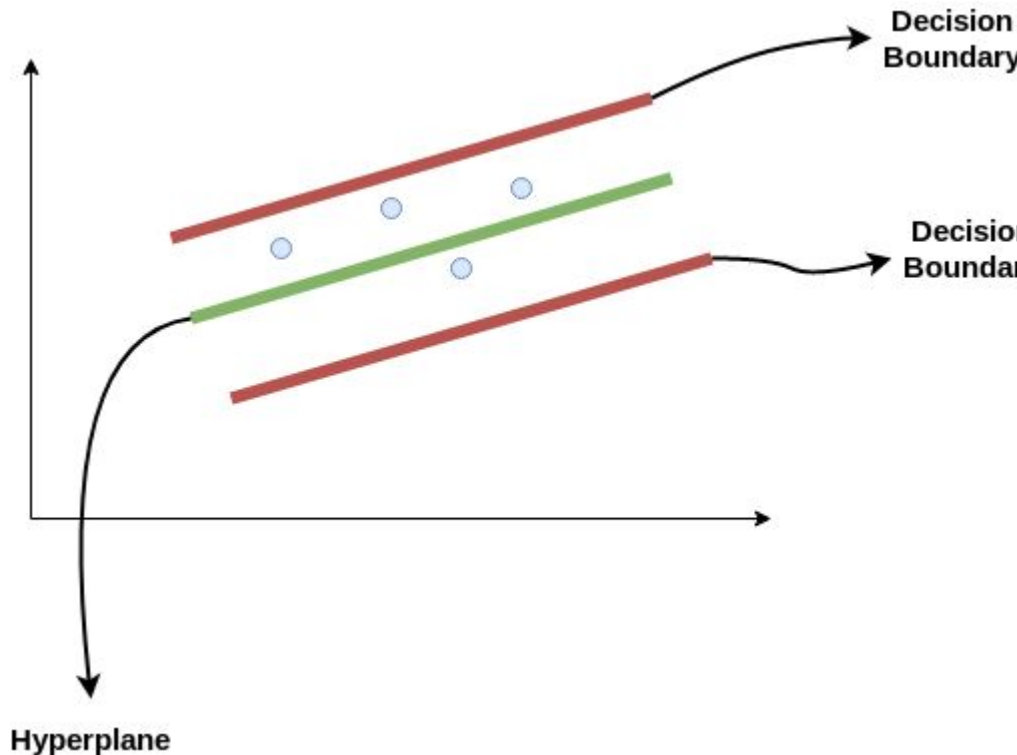INPUTS   OUTPUTS

Method - Build models

- First Regression Task - Predict Mechanical properties
- Models used:
  - Support Vector Regressor
  - Artificial Neural Networks
  - XGBoost Regressor

Support Vector Regressor

- Works on the principle of Support Vector Machines(SVM).
- To find a decision boundary such that data points closest to hyperplane are within that boundary line
- We are going to take only those points that are within the decision boundary and have the least error rate.

Neural Net

- Input layer contains the compositions of the Mg alloy AND the processing condition of the alloy

- Outputs the properties of Mg Alloy.

  - For eg

UTS   YS   Ductility

432   397   11.4
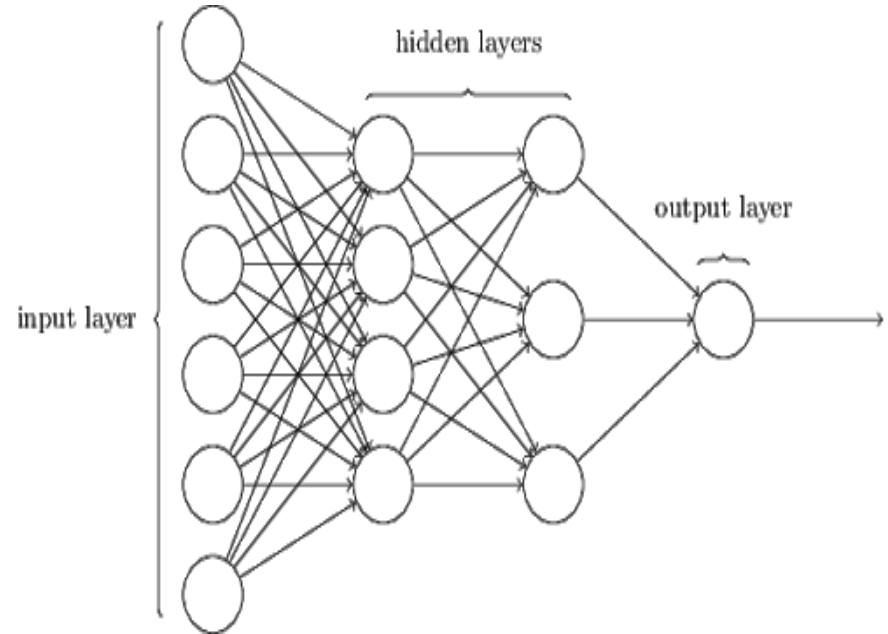
XGBoost-Regressor

- Boosting is an ensemble technique where new models are added to correct the errors made by existing models. Models are added sequentially until no further improvements can be made.

- Gradient boosting is an approach where new models are created that predict the residuals or errors of prior models and then added together to make the final prediction

> " *When in doubt, use xgboost.*
>
> — Avito Winner's Interview: 1st place, Owen Zhang

- It is called gradient boosting because it uses a gradient descent algorithm to minimize the loss when adding new models.

- Works well with small datasets and sparse datasets.

Results from our models
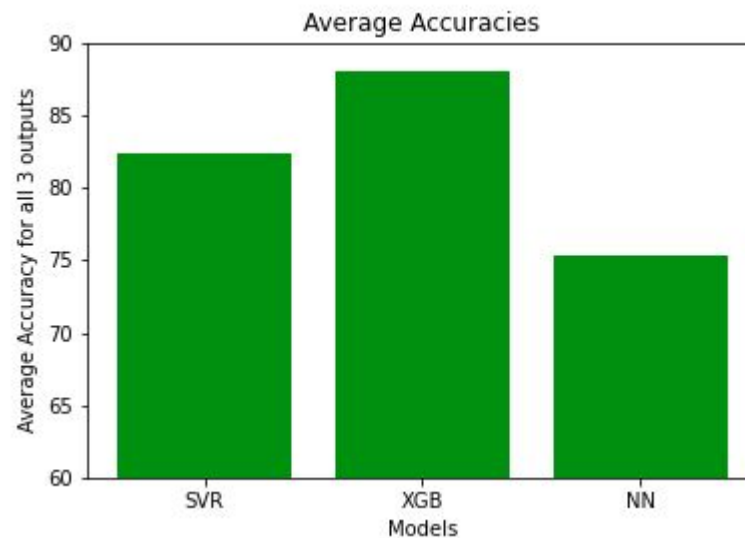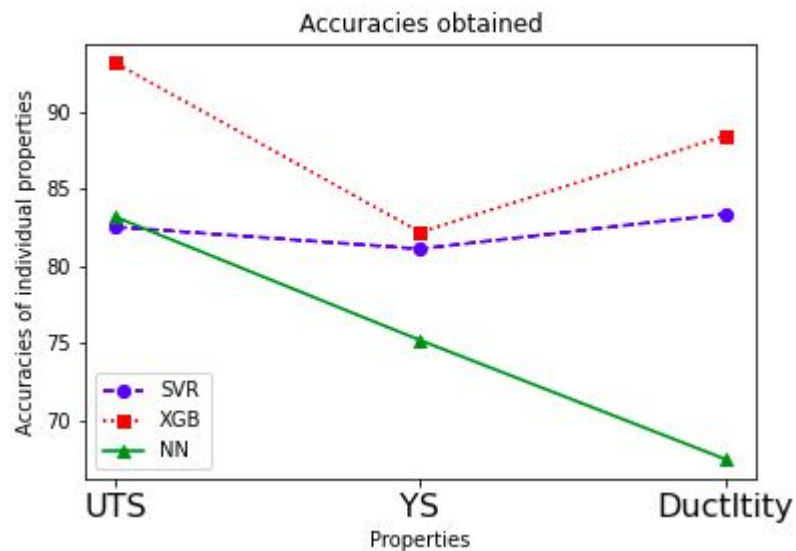
Method - Find composition

- Our main goal is to find a Mg alloy composition that have desirable mechanical properties which can be used to create lightweight vehicles and have strong qualities.
- What we have till now:
  - Data available
  - Trained model that predicts mechanical properties
- What we want :
  - An optimum alloy composition that gives desirable mechanical properties.

Method-Find composition

- Create Synthetic data that generates data samples present in the feature space of our training data.
- Create Randomly generated data following the restrictions of each element.
- Use the data generated as our training samples and predict the properties using our trained model.

What is an ideal Mg alloy?

- An ideal Mg alloy should have the following properties
  - Alloy's Ultimate Tensile Strength(UTS) > Alloy's Yield Strength(YS)
  - UTS > 400 (400-500)
  - Ductility >10 (10-15)
- The generated Mg alloy should have these ideal properties.

An example of an alloy designed using ML

Mg	Al	Zn	Mn	Ce	La	Nd	....	UTS	YS	Duct
95.652124	0	0.910634	0	0	0.0468075	0	......	485.73535	410.19900	13.823895
85.041531	5.027281	4.953463	0.001893	0.016910	0.009582	4.949043	....	425.00302	407.64773	13.263954

Conclusion

- New alloy design and Discovery!
- Significant research is still needed on magnesium processing, alloy development, joining, surface treatment, corrosion resistance and mechanical properties improvement to achieve future goals to reduce the vehicle mass and the amount of greenhouse gases.
- Production and application technologies must be cost effective for magnesium alloys to make magnesium alloys an economically viable alternative for the automotive industry.