Computational Material Design and Discovery of Magnesium Alloys.

Samyak Jain
Supervisor : Nick Birbillis
The Australian National University
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.
Motivation

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

- **Engine:** Mg = 16 kg, Al = 22 kg, Wt. Reduction = 22 to 70%
- **Door inner:** Mg = 5.4 kg, Al = 8.2 kg, Wt. Reduction = 33%
- **Steering wheel core:** Mg = 0.9 kg, Steel = 1.4 kg, Wt. Reduction = 33%
- **Steering column:** Mg = 1.4 kg, Steel = 2.3 kg, Wt. Reduction = 40%
- **Lift gate:** Mg = 3.2 kg, Al = 5.5 kg, Wt. Reduction = 42%
- **Instrument panel:** Mg = 1.8 kg, Steel = 5 kg, Wt. Reduction = 64%
- **Transfer case:** Mg = 11.4 kg, Steel = 15.6 kg
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 Ductility, Tensile Strength and Yield Strength.
- Use of Machine learning to predict these properties.
Method - Data Mining

1. Identify good sources
2. Remove noise
3. Apply algorithms
4. Explain results and take actions

- Data collection
- Data cleaning
- Data analysis
- Interpretation
Data Mining

- MATWEB - Professional Material search Web
- CES Material Selection
- Journal Articles
- Research Papers
- Google Scholar
### What the data looks like

<table>
<thead>
<tr>
<th></th>
<th>Name</th>
<th>Condition</th>
<th>Condition (Numeric)</th>
<th>Mg</th>
<th>Al</th>
<th>Zn</th>
<th>Dy</th>
<th>Fe</th>
<th>UTS</th>
<th>YS</th>
<th>Ductility</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Mg-Zn-Ho</td>
<td>Extrusion</td>
<td>230 degree C</td>
<td>1</td>
<td>93</td>
<td>0</td>
<td>6</td>
<td>0</td>
<td>280</td>
<td>200</td>
<td>15</td>
</tr>
<tr>
<td>B</td>
<td>Mg-Zn-Ho</td>
<td>Extrusion</td>
<td>210 degree C</td>
<td>1</td>
<td>96.9</td>
<td>0</td>
<td>2.7</td>
<td>0</td>
<td>208</td>
<td>300</td>
<td>20</td>
</tr>
<tr>
<td>C</td>
<td>AZ61-A2</td>
<td>Extrusion</td>
<td></td>
<td>1</td>
<td>92.23</td>
<td>6.76</td>
<td>0.74</td>
<td>0</td>
<td>297</td>
<td>319</td>
<td>18</td>
</tr>
<tr>
<td>D</td>
<td>AZ80-39</td>
<td>Extrusion</td>
<td></td>
<td>1</td>
<td>90.66</td>
<td>8.4</td>
<td>0.6</td>
<td>0</td>
<td>329</td>
<td>333</td>
<td>13</td>
</tr>
</tbody>
</table>

- 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

\[ \text{Inputs} + \text{Outputs} = \text{The alloy properties} \]
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
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.

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

<table>
<thead>
<tr>
<th>Mg</th>
<th>Al</th>
<th>Zn</th>
<th>Mn</th>
<th>Ce</th>
<th>La</th>
<th>Nd</th>
<th>UTS</th>
<th>YS</th>
<th>Duct</th>
</tr>
</thead>
<tbody>
<tr>
<td>95.65212</td>
<td>0</td>
<td>0.91063410</td>
<td>0</td>
<td>0.046807</td>
<td>0</td>
<td></td>
<td>485.7353</td>
<td>410.1990</td>
<td>13.823895</td>
</tr>
<tr>
<td>85.04153</td>
<td>5.027281</td>
<td>4.953463</td>
<td>0.001893</td>
<td>0.016910</td>
<td>0.009582</td>
<td>4.949043</td>
<td>425.003</td>
<td>407.6477</td>
<td>13.263954</td>
</tr>
</tbody>
</table>
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.
THANK YOU!