Research Objective – Create a reliable system to derive compositions of alloys with desirable physical properties such as tensile strength and thermal conductivity, using machine learning tools.

State of the art –

* Use NN architecture to get good and reliable results along with inverse modelling.
  + Do not provide a system/tool to reproduce results or use their research
* Data for copper alloys and properties is accessible, but mass evaluation is not easy, in the current state.

Background

* Copper alloys
* Machine learning
* Tensile strength
* Thermal Conductivity/Electrical conductivity
* Data Pre-processing
* Random forests
* Regression problems
* Supervised learning
* Data collection
* Principal Component Analysis
* K-nearest neighbors regression
* K-fold cross validation
* Train-test split
* Hyperparameter Optimisation

Methodology

* Data Collection
* Exploratory Data Analysis
* Data Pre-processing (different for TS and TC)
* Model Selection
* Hyperparameter Tuning
* Model evaluation
* Model freezing
* Inverse predictions (i.e. alloy composition from value of property)
  + Select best samples
  + Generate combinations of compositions from best samples
  + Make predictions
  + Return compositions with predictions closest to desired value
  + Comparing generated predictions to the values in data