

- Heat treatment conditions - temperature, time and other process conditions for normalizing, through-hardening, carburizing-quenching and tempering processes
- Mechanical properties - YS, UTS, %EL, %RA, hardness, Charpy impact value (J/cm²), fatigue strength.

The data used in this work has 437 instances/rows, 25 features/columns (composition and processing parameters), and 1 target property (fatigue strength). The 437 data instances include 371 carbon and low alloy steels, 48 carburizing steels, and 18 spring steels. This data pertains to various heats of each grade of steel and different processing conditions. The details of the 25 features and given in Table 1.

Methods

The overall proposed approach is illustrated in Figure 1. The raw data is preprocessed for consistency using domain knowledge. Ranking-based feature selection methods are also used to get an idea of the relative predictive potential of the attributes. Different regression-based predictive modeling methods are then used on the preprocessed and/or transformed data to construct models to predict the fatigue strength, given the composition and processing parameters. All constructed models are evaluated using Leave-One-Out Cross Validation with respect to various metrics for prediction accuracy. Below we present the details of each of the 4 stages.

Table 1 NIMS data features

Abbreviation	Details
C	% Carbon
Si	% Silicon
Mn	% Manganese
P	% Phosphorus
S	% Sulphur
Ni	% Nickel
Cr	% Chromium
Cu	% Copper
Mo	% Molybdenum
NT	Normalizing Temperature
THt	Through Hardening Temperature
THt	Through Hardening Time
THQCr	Cooling Rate for Through Hardening
CT	Carburization Temperature
Ct	Carburization Time
DT	Diffusion Temperature
Dt	Diffusion time
QmT	Quenching Media Temperature (for Carburization)
TT	Tempering Temperature
Tt	Tempering Time
TCr	Cooling Rate for Tempering
RedRatio	Reduction Ratio (Ingots to Bar)
dA	Area Proportion of Inclusions Deformed by Plastic Work
dB	Area Proportion of Inclusions Occurring in Discontinuous Array
dC	Area Proportion of Isolated Inclusions
Fatigue	Rotating Bending Fatigue Strength (10⁷ Cycles)