Decoding the genome of cement by Gaussian Process Regression

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Background and motivations

- Concrete (and cement) represents a typical engineering material that involves a heavy carbon footprint
- Top-one produced engineering material in human history
- Concrete is extensively used in modern construction

Concrete constructions and the environmental issues behind

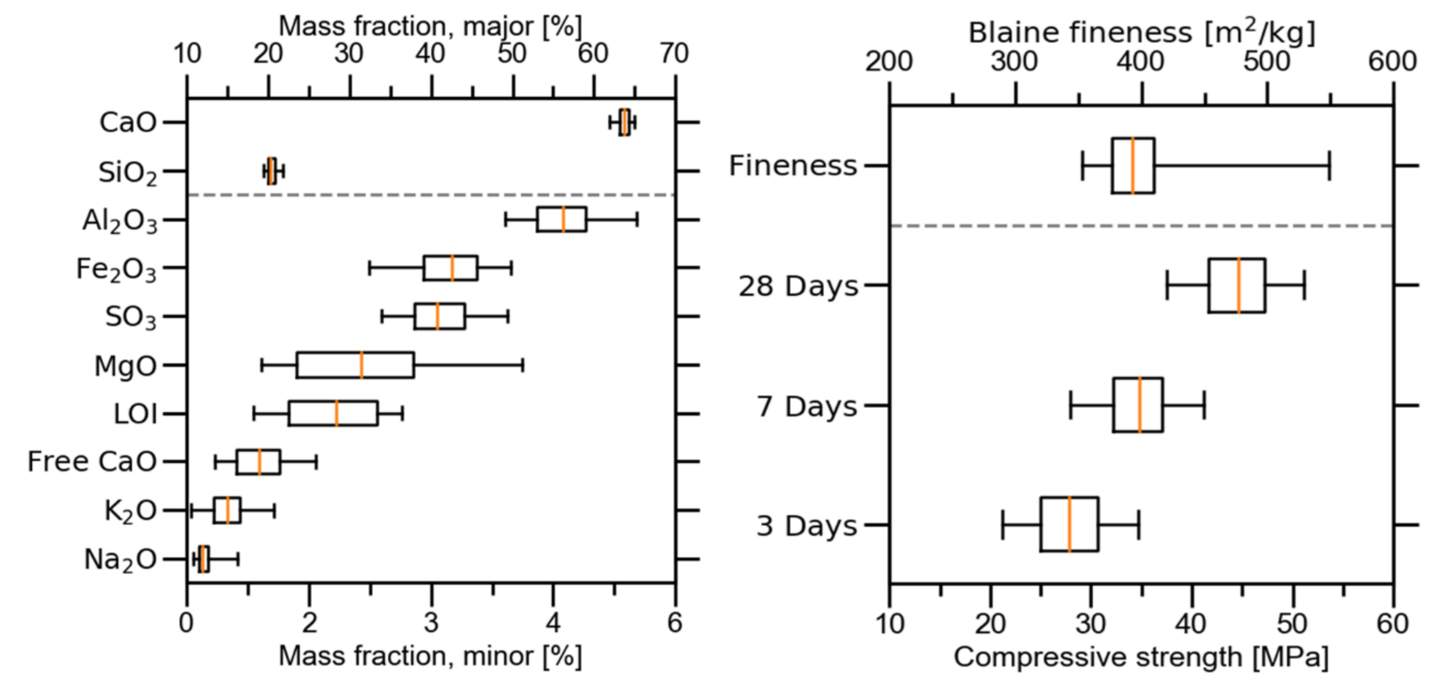
- Cement is a complex composite of physical and chemical phases formed by various oxides (i.e., the cement "genome")
- 1-ton cement ≈ 1-ton CO_2 and 4×10^9 tons produced annually
- Need to improve strength performance and reduce the carbon embodiment of cement
- Challenges: identify the effect of each oxide compounds
- A good manifestation of the common difficulties faced by many studies in engineering materials

Methods

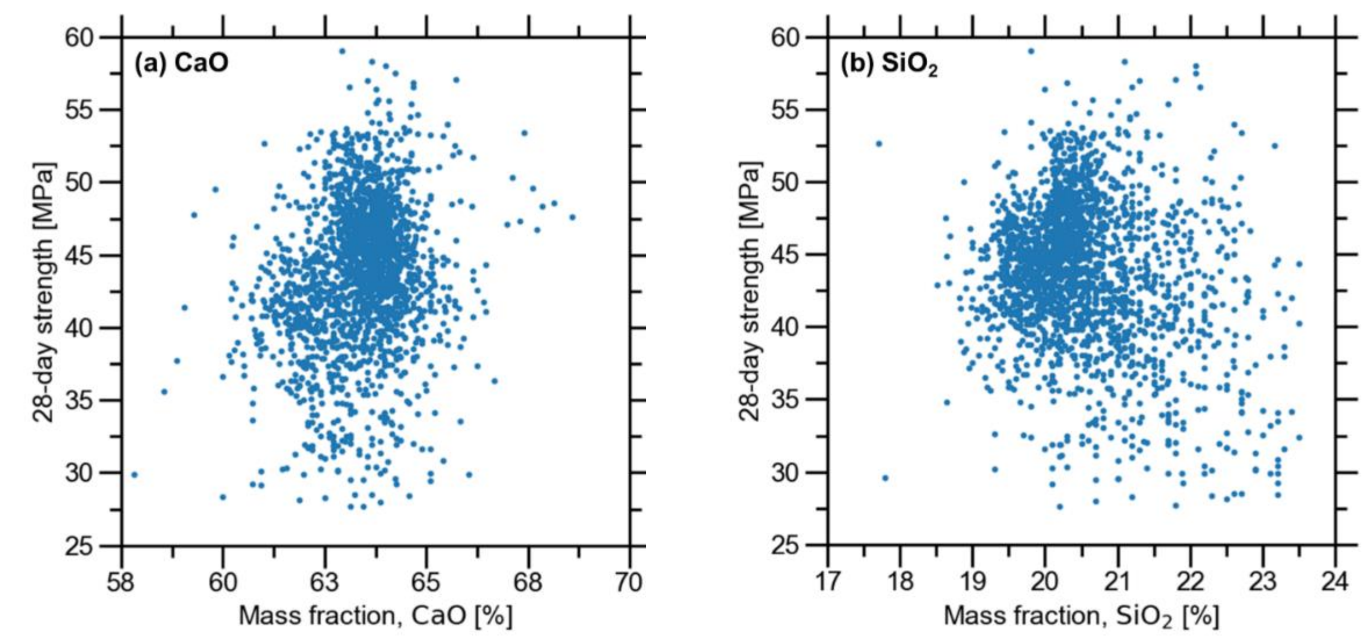
- Machine learning is more used to predict material properties
- This study aims to apply Gaussian process regression (GPR) to explain the composition-strength relationship of cement
- GPR is adopted because of several advantages:
  1. Non-parametric: good model flexibility
  2. Leveraging the prior knowledge via kernel selection
  3. Uncertainty estimation of the prediction: practical for the rational design of engineering materials

The cement dataset

- This dataset is collected over many U.S. cement testing institutes, consisting of 2060 cement samples
- Input features: oxide contents (CaO, SiO_2, etc.) and fineness
- Output target: 28-day strength (i.e., the standard reference)



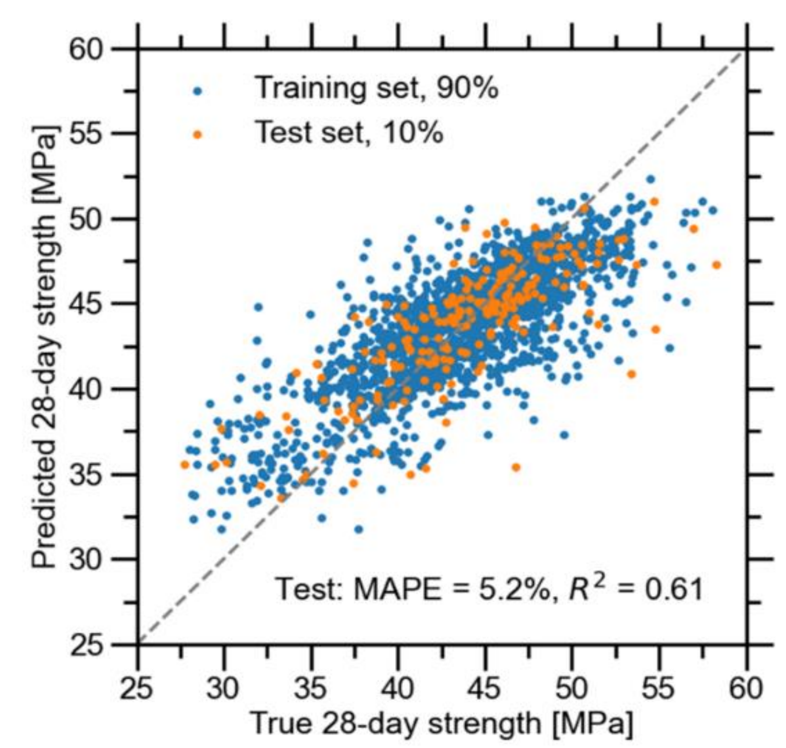
Variation of each item in the dataset.



No correlation between the strength and input features

GPR optimization and accuracy

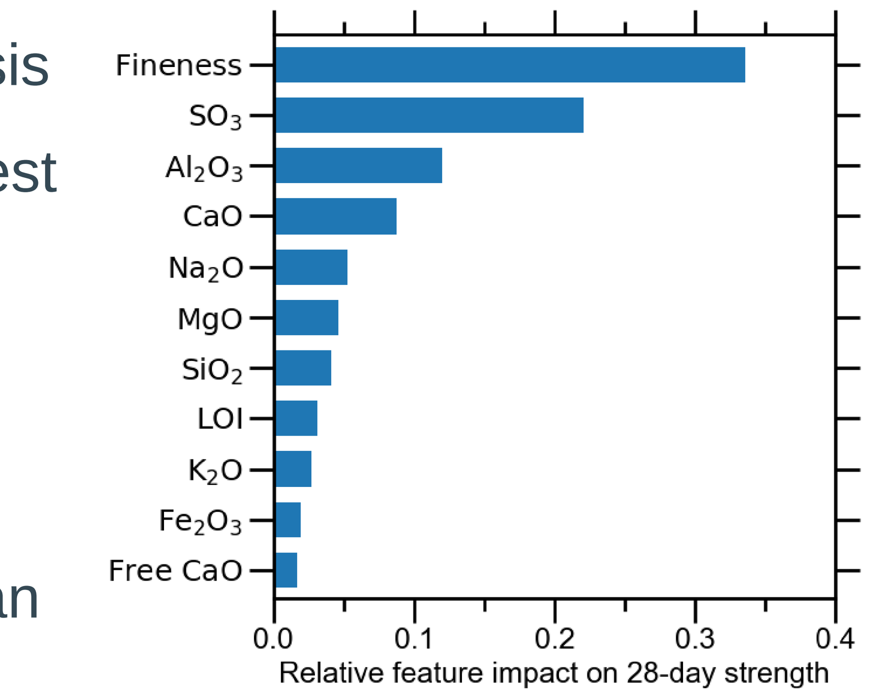
- [Linear + RBF] as the best kernel
- Noise is tuned for overfitting
- Test: 10% stratified samples
- The highest accuracy ever reported on this dataset
- An illustration of the common challenges for studying



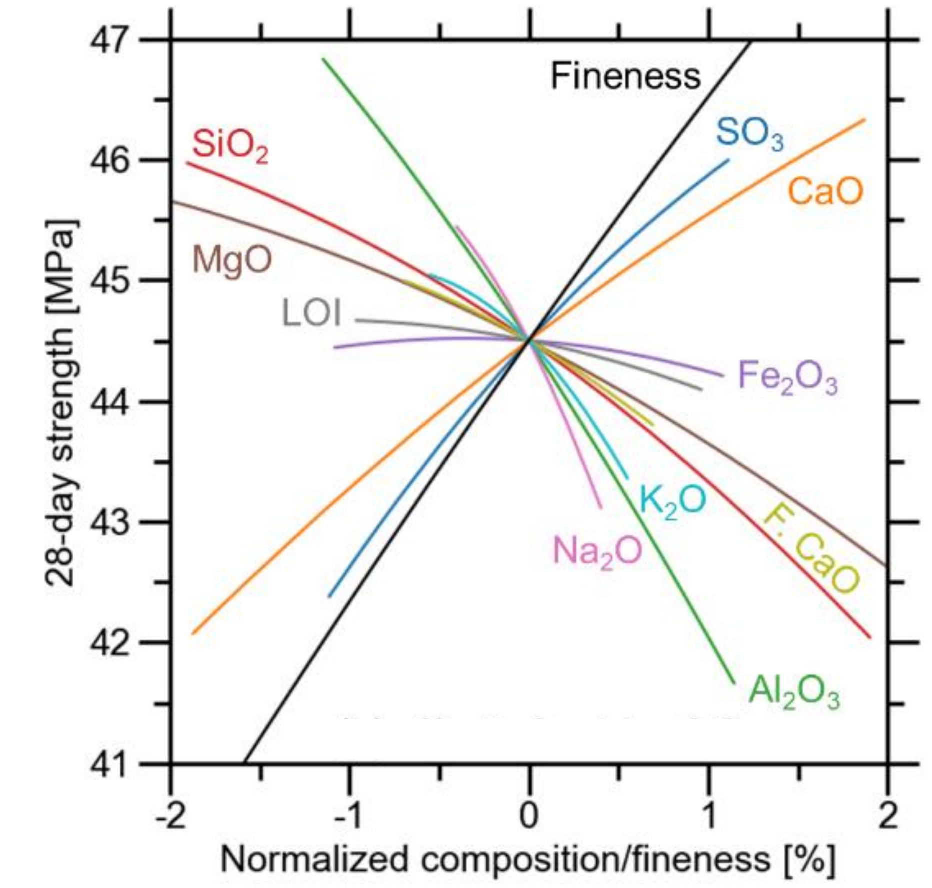
Predicted vs. true strength

Interrogation on the trained model

- The first feature impact analysis is based on the permutation test
- This analysis focuses on the magnitude of the influence
- The rank highlights that the fineness is more important than any oxide

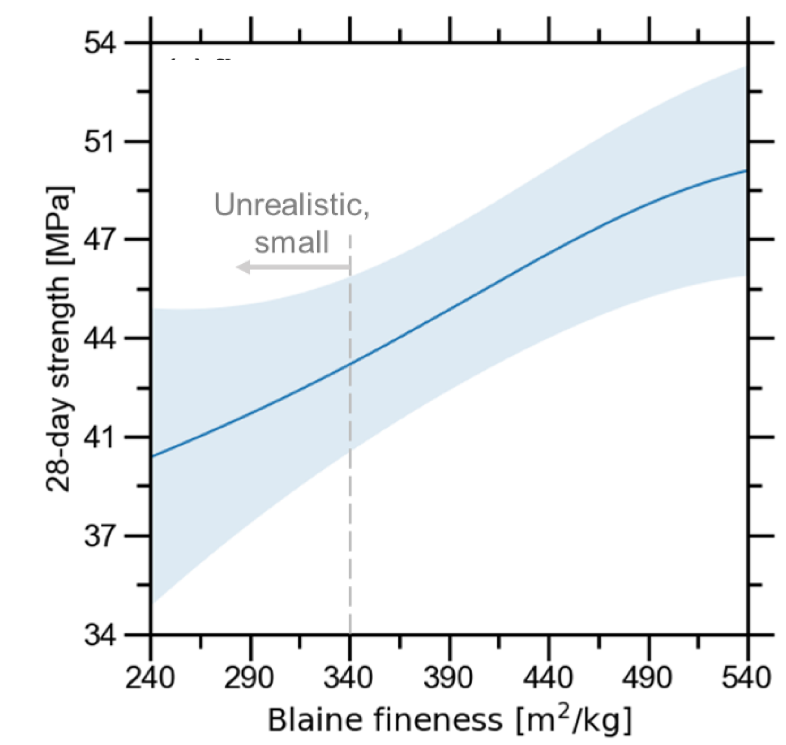


Feature impact analysis



Feature effect analysis

- Feature effect analysis
- Tune only one feature from its min to max
- The trends of the major oxides are broadly in line with cement chemistry
- Important insight for high-performance cement



Uncertainty for Fineness

- Uncertainty of GPR prediction
- The shadowed region represents the standard deviation
- The high uncertainty for small fineness is due to limited sample
- The awareness of uncertainty is very practical for the design of engineering materials

Remarks: The presented archetypal pipeline successfully maps the material property, and it can be applied to advance the study, design, and optimization of many other materials

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