# Materials Informatics Approach to Predictive Models for Elastic Modulus of Polypropylene Composites

Y. Araki, Y. Ikeda, M. Okuyama, Y. Nakazawa, T. Oshiyama and K. Funatsu
KONICA MINOLTA, Inc., Hachioji, Tokyo, Japan
Department of Chemical System Engineering, The University of Tokyo, Bunkyo-ku, Tokyo, Japan
Nara Institute of Science and Technology, Ikoma, Nara, Japan

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## Introduction

**Example application of composites**
- **Battery module covers**
- **Interior materials of aircraft**
- **Interior materials of automobile**

**...**

**Three elemental materials of composites**

Polymer (PP) | Filler | Additive

**Vast number of combinations among these materials**
⇓
**Almost unable to consider all of them by human**
⇓
**Machine learning method can be useful to obtain valuable candidates for measurement**

**However, the detail information (physical property etc…) of these components are often NOT-acquirable in an actual corporate research.**

## Purpose

**To establish a machine learning method to predict target properties by using only categorical information**

**Information about brand names**
**Base polymer** : $m_1, m_2, m_3, \dots$
**Additive** : $a_1, a_2, a_3, \dots,$
**Filler** : $f_1, f_2, f_3, \dots,$

**Machine Learning**

**Target Property**
Ex. Elastic modulus, etc...

## Method

### 1. Featurizing formulation of composites

Experimental setting in this research

| Target Property | Control Parameter | | |
|---|---|---|---|
| Elastic Modulus | PP | Additive | Filler |
| | 11 | 17 | 20 |

| | Recipe of a composite | | |
|---|---|---|---|
| Component | PP | Additive | Filler |
| Name | $m_i$ ( $i$ = 1-11 ) | $a_j$ ( $j$ = 1-17 ) | $f_k$ ( $k$ = 1-20 ) |
| Mass ratio | 1 | $x_{aj}$ | $x_{fk}$ |

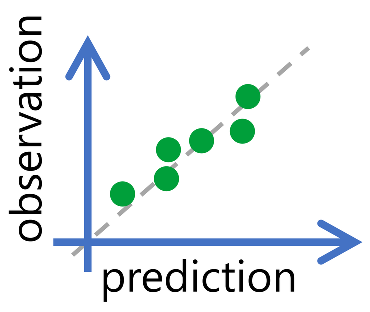
Representing a recipe by using dummy variables

$$\boldsymbol{x} = (\underbrace{0, \dots, \underset{i}{1}, \dots, 0}_{11}, \underbrace{0, \dots, \underset{j}{x_{aj}}, \dots, 0}_{17}, \underbrace{0, \dots, \underset{k}{x_{fk}}, \dots, 0}_{20})$$

We use this $\boldsymbol{x}$ as a feature to predict an elastic modulus.
The dimension of $\boldsymbol{x}$ : 11 + 17 + 20 = 48.

### 2. Partial Least Square (PLS) Method

Dummy variable representing a recipe $\boldsymbol{x}$ → PLS → Predicted elastic modulus $\boldsymbol{y}$



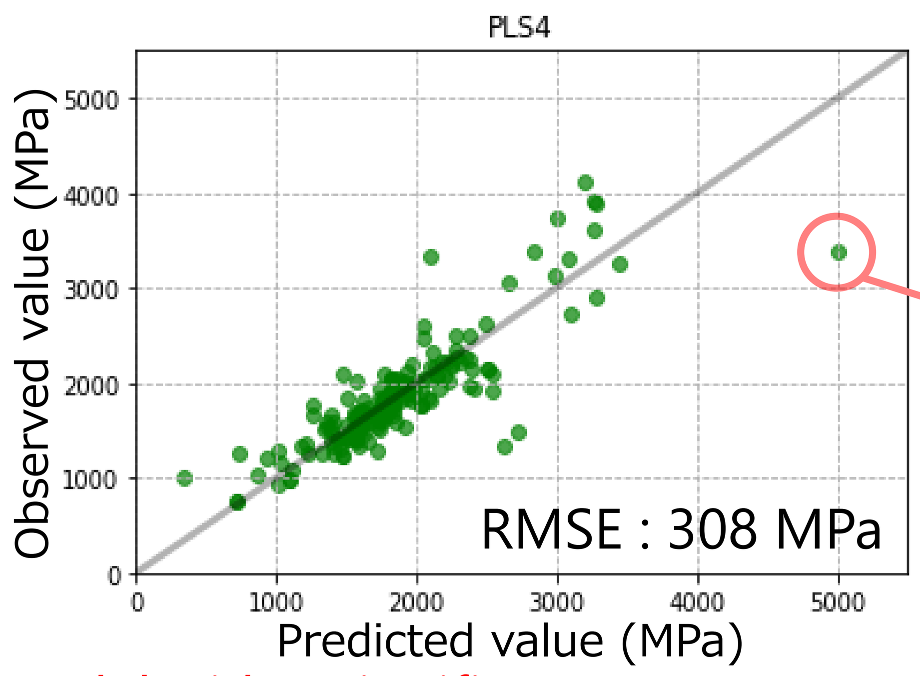

### 3. Evaluation & Analysis

1. Evaluating constructed PLS model by predicting test data
⇓
2. Performing actual experiment to check prediction results
⇓
3. Analyzing the experimental results comparing the model prediction

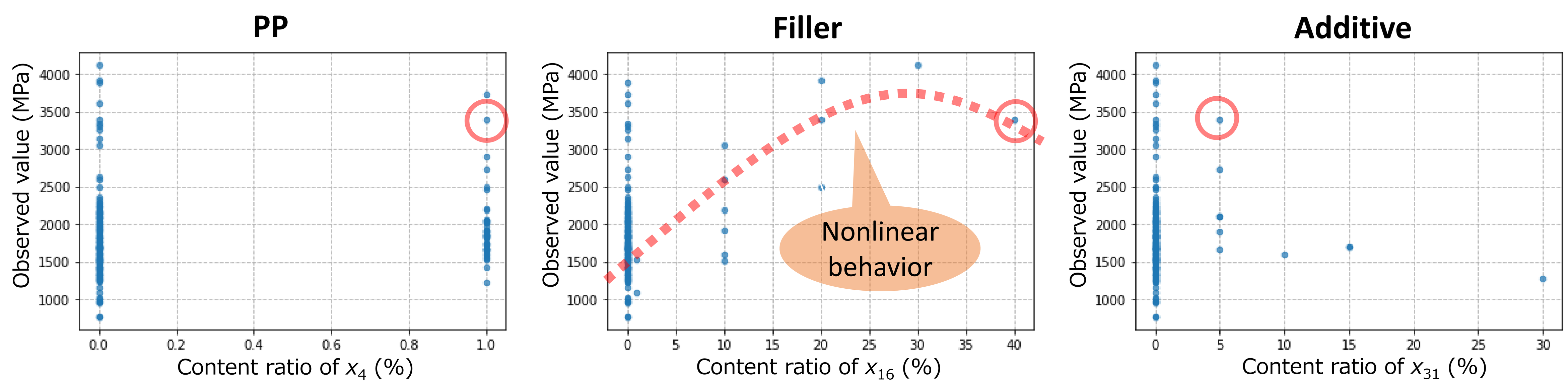
## Result & Discussion

### The result of PLS regression for elastic modulus

※ The hyperparameter of PLS was optimized by LOOCV




The model with a significant accuracy was constructed.
However, a few data points were outlier (red circle).



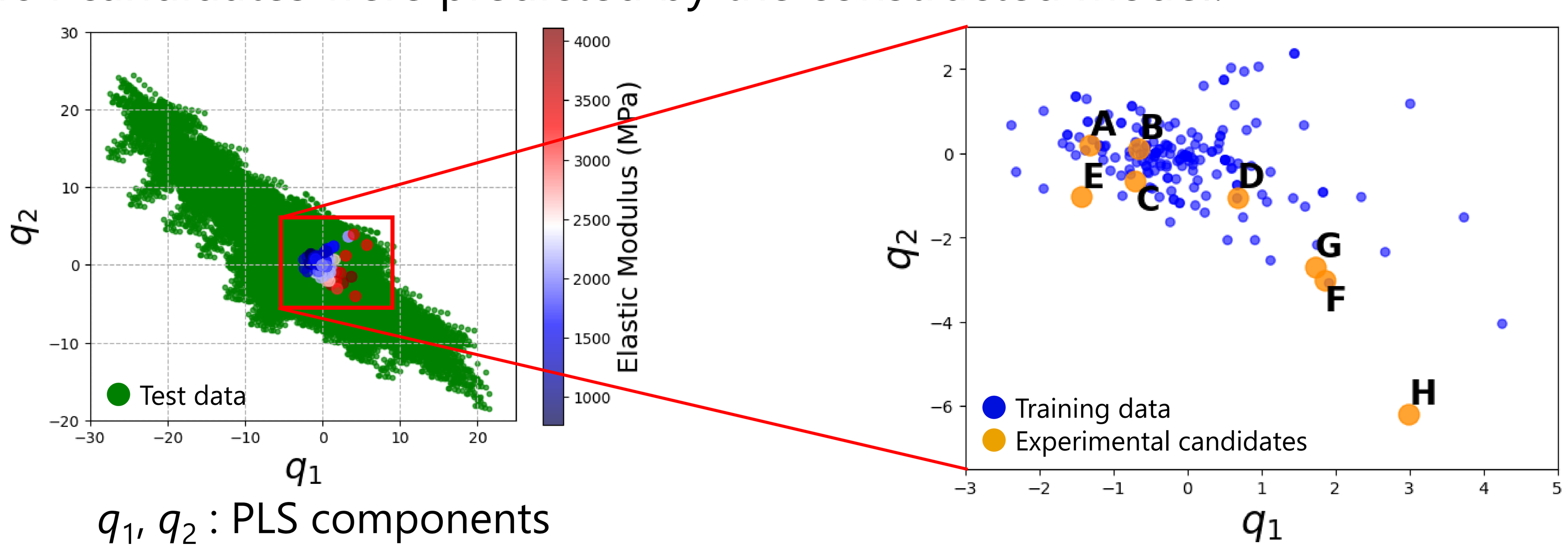

| Material | PP | Filler | Additive |
|---|---|---|---|
| Component | $x_4$ | $x_{16}$ | $x_{31}$ |
| Ratio | 55 | 40 | 5 |

PLS : **Linear** regression model
⇕
The observed elastic modulus behaves **non-linearly** against $x_{16}$ value.

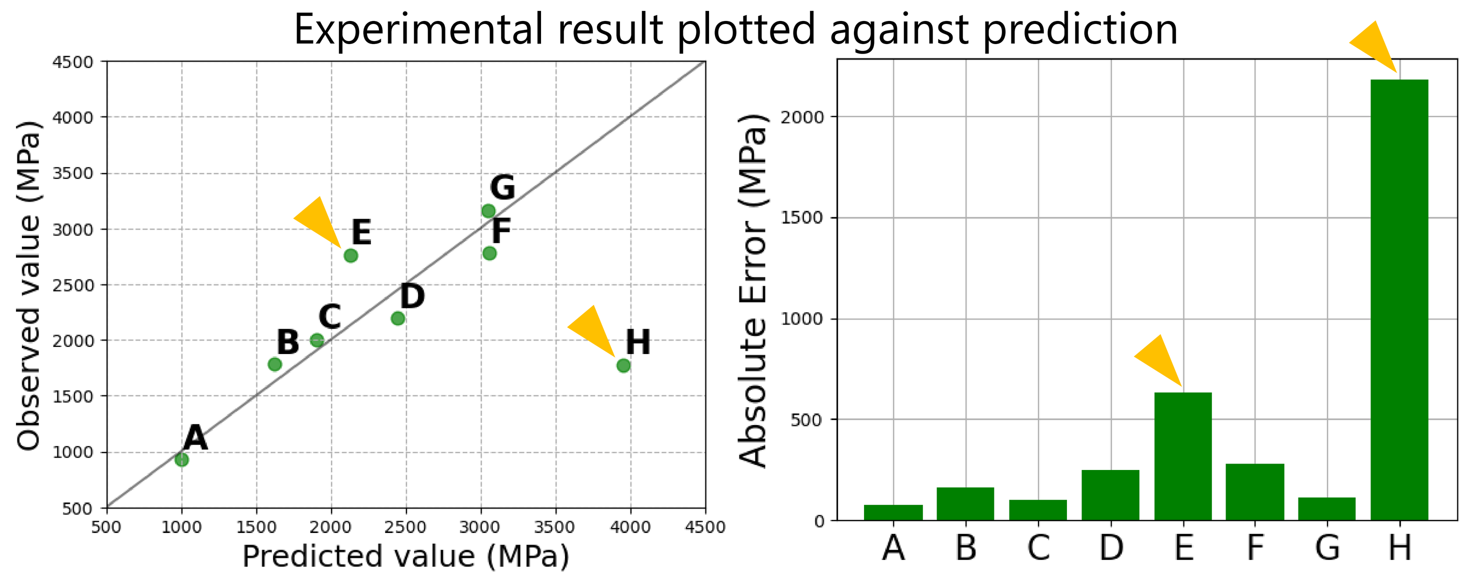
The constructed model can not predict this data point because of non-linearity for content ratio.

### Evaluating test data by performing actual measurement

575484 candidates were predicted by the constructed model.

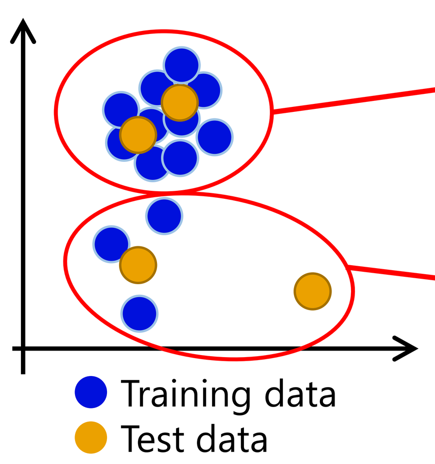



$q_1$, $q_2$ : PLS components




The prediction errors of E & H were relatively large.
H ⇒ **Far away** from training data as well as the above case.
E ⇒ **Sparse** training data points

Summering these results...




Around a lot of training data...
⇒ **Possibly well-predicted !**

Sparse training data points or almost nothing...
⇒ **Low prediction accuracy...**

## Conclusion & Future Work

1. Elastic property of composites can be predicted by using only categorical information of materials.
   ⇒ We can obtain valuable recipes from vast number of candidates.
2. The prediction accuracy can be checked by visualizing a feature space of a regression model.
   ⇒ To evaluate the reliability of the prediction, a Bayesian approach will be applied.

To consider the interaction between materials for more precise prediction…
⇒ **See poster #1130** & "M. Okuyama *et al.*, Sci. Technol. Adv. Methods., **2**, 1, 106-118 (2022)."