Applications of machine learning in material research: an overview

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Outlines

1 Introduction to AI & machine learning
2 Some typical applications of machine learning
3 Challenges & solutions
4 Conclusions
Artificial intelligence (AI): techniques that enable computers mimic human intelligence

Human intelligence: Imagination, creativity, fantasy, intuition, problem solving

Machine learning (ML): historical data (input X, output Y) is used to derive functional relationship $Y=f(X)$ and apply it for future data predictions. Data fitting

Input X: 1D structured data (e.g. excel data sheet)
- 2D image
- time serial sequence

Output Y: categorical labels (classification)
- continuous values (regression)

Conventional machine learning: manual feature engineering before training

Deep learning (DL): learn directly from raw data without manual feature engineering
MSE data — AI models — PSP relationship

AI is a universal tool
Predicting properties of steel plate

10000+ Real-factory data (excel data sheet)
1 hidden layer shallow neural network

Input:
Composition, Heating temperature, Thickness, Rolling velocity, etc.

Output:
Yield strength, Tensile strength, Elongation, $\sigma_s/\sigma_b$, Drop weight tear testing

$10000+ \text{Real-factory data (excel data sheet)}$
$1 \text{hidden layer shallow neural network}$

Input Layer
- C
- Si
- Mn
- $x_i$
- $x_n$

1st Hidden Layer
- $h_1$
- $h_2$
- $h_m$

Output Layer
- $y$

$y = \sum_{i=1}^{m} W_{1i}^{(2)} h_i^{(1)} + b_1^{(2)}$

$1 \text{hidden layer shallow neural network}$

High training & testing accuracy
0.99 (Pearson coefficient of prediction and real data)
Predicting solidification cracking susceptibility of stainless steel

Dataset size: 487*22 matrix

Varestraint SCS test: include composition factors, processing parameters, and strain
Total crack length (TCL): indicator for SCS
21 input: composition and test parameters
1 output: the indicator for solidification cracking susceptibility TCL (total crack length)
Predicting glass-forming ability

Dataset size: 10440 entries
Input: composition
Output: GFA

MF: 1-D vector
PTR: 2-D image

SNN
CNN

Binary, ternary, etc.

10000+ data collected from literature

None: not able to form metallic glass
Ribbon: able to form thin (20-30μm) metallic glass
BMG: able to form thick metallic glass (1 mm)

Input: alloy composition

3 labels: None, Ribbon, BMG
Defect detection

Online, high speed (>10m/s), high temperature (>1000 °C) metal products’ surface quality inspection


2-class classification (OK vs. NOK)

<table>
<thead>
<tr>
<th>Feature extraction</th>
<th>Classifier</th>
<th>AUC</th>
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<tbody>
<tr>
<td>LBP features</td>
<td>SVM</td>
<td>0.92</td>
</tr>
<tr>
<td>LBP features</td>
<td>Random Forests</td>
<td>0.95</td>
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<tr>
<td>CNN-SURFIN</td>
<td>Commercial (SVM)</td>
<td>0.997</td>
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<table>
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<tr>
<th></th>
<th># images</th>
<th>Defect type</th>
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<tbody>
<tr>
<td>OK</td>
<td>2475</td>
<td></td>
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<tr>
<td>NOK</td>
<td>1411</td>
<td>315 Rol Mark</td>
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<tr>
<td></td>
<td></td>
<td>887 Folds</td>
</tr>
<tr>
<td></td>
<td></td>
<td>209 Cracks</td>
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<tr>
<td>TOTAL</td>
<td>3886</td>
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Defect detection on an X-ray image of a jet turbine blade

The training dataset did not contain any turbine blade images.

Microstructure recognition

Martensite: red
Tempered martensite: green
Bainite: blue
Pearlite: yellow

Challenges & Solutions

1. Small dataset - Data augment
2. Imbalanced data distribution – Add weight to data
3. Noise in data - Regularization
4. Poor interpretability of black box models - Combine different models together & Visualization
5. Lack proper descriptors - Exploit deep learning
6. Poor accuracy - pre-training
Regularization

To improve generalization, add msw (mean square weight) to simple loss function $J(\theta)$ e.g. mse (mean square error)

$$\text{mse} = \frac{1}{N} \sum_{i=1}^{N} (e_i)^2 = \frac{1}{N} \sum_{i=1}^{N} (t_i - a_i)^2$$

$$\text{msw} = \frac{1}{n} \sum_{j=1}^{n} W_j^2$$

$$J(\theta) = \text{msereg} = \gamma \text{mse} + (1 - \gamma) \text{msw}$$

$$\Theta^1 = \Theta^0 - \alpha \nabla J(\Theta) \quad \text{evaluated at } \Theta^0$$

Backpropagation algorithm
Black box models?

Tree-based models: good interpretability

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**Tree-based models**

- **Ni ≤ 15.085**
  - **mse = 17.609**
  - **samples = 487**
  - **value = 3.846**

- **Strain ≤ 2.75**
  - **mse = 8.529**
  - **samples = 297**
  - **value = 2.36**

- **Ve ≤ 4.215**
  - **mse = 11.249**
  - **samples = 104**
  - **value = 4.153**

- **Ni ≤ 10.8**
  - **mse = 4.398**
  - **samples = 193**
  - **value = 1.394**

- **Strain ≤ 0.75**
  - **mse = 22.703**
  - **samples = 190**
  - **value = 6.168**

- **Ve ≤ 1.29**
  - **mse = 21.736**
  - **samples = 131**
  - **value = 7.7**

- **Th ≤ 4.09**
  - **mse = 8.072**
  - **samples = 59**
  - **value = 2.767**

- **Ve = 17.422**
  - **samples = 104**
  - **value = 9.074**

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**Graph showing feature importance**

- **Feature's importance**
  - **Ni**
  - **Strain**
  - **C**
  - **Mo**
  - **N**
  - **Si**
  - **Ti**
  - **P**
  - **S**
  - **Ve**
  - **I**
  - **Co**

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**EPSRC**

Engineering and Physical Sciences Research Council.
Exploit deep learning

PTR (periodical table representation): mapping each composition to the periodical table forming a 9*18 gray image

Only composition is needed to predict glass-forming ability

Input $\rightarrow$ 3*3/Conv/8 filter $\rightarrow$ max pooling $\rightarrow$ 3*3/Conv/16 filter $\rightarrow$ max pooling $\rightarrow$ 3*3/Conv/32 filter $\rightarrow$ max pooling $\rightarrow$ flatten $\rightarrow$ FC $\rightarrow$ softmax

CNN’s average accuracy (10 cross validation): 96.7% (train)/95.8% (test)
Pretraining to improve accuracy

Deep neural network initiation using stacked auto-encoders (i.e. pretraining)

Stacked auto-encoders provide optimized initial W and b to deep neural network
Conclusions

1 AI & Machine learning:
   a powerful universal tool for accelerating the
development of materials;
an important supplement to theory and experiments.

2 Though there are many challenges when solve
materials problems using machine learning, solutions exist.
Thank you!