IMPaCT

EPSRC Centre for Doctoral Training in Innovative Metal Processing (IMPaCT)

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

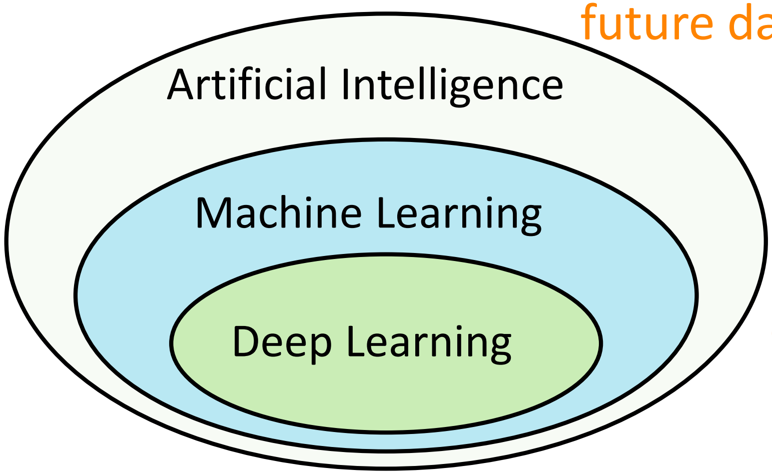
4 Conclusions

AI, ML, DL

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

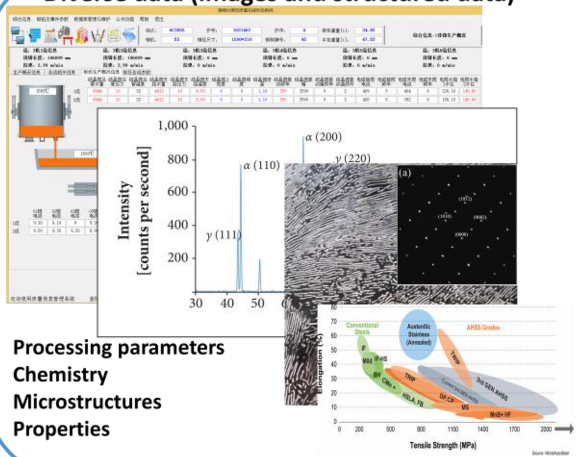
Output Y: categorical **labels** (classification)
continuous **values** (regression)

Conventional machine learning: **manual feature engineering** before training

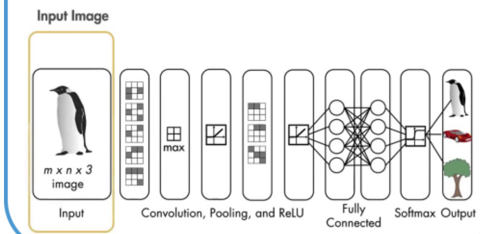
Deep learning (**DL**): **learn directly from raw data** without manual feature engineering

MSE data — AI models — PSP relationship

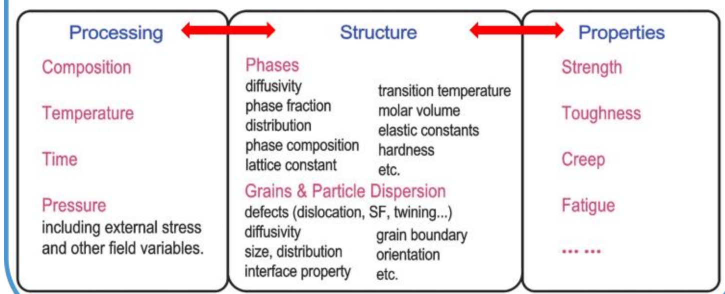
Diverse data (images and structured data)

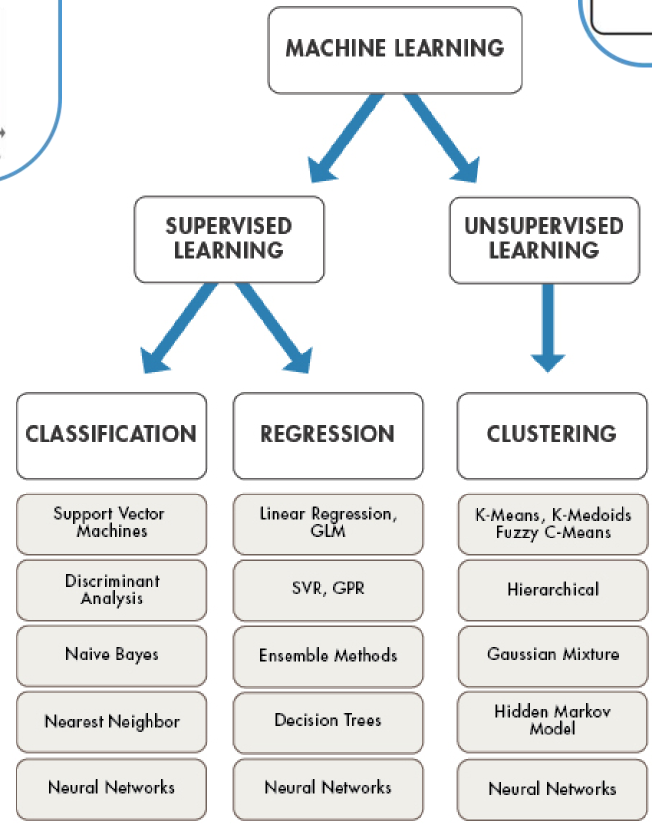


AI models



P-S-P relationship used in material design





AI is a universal tool

Predicting properties of steel plate

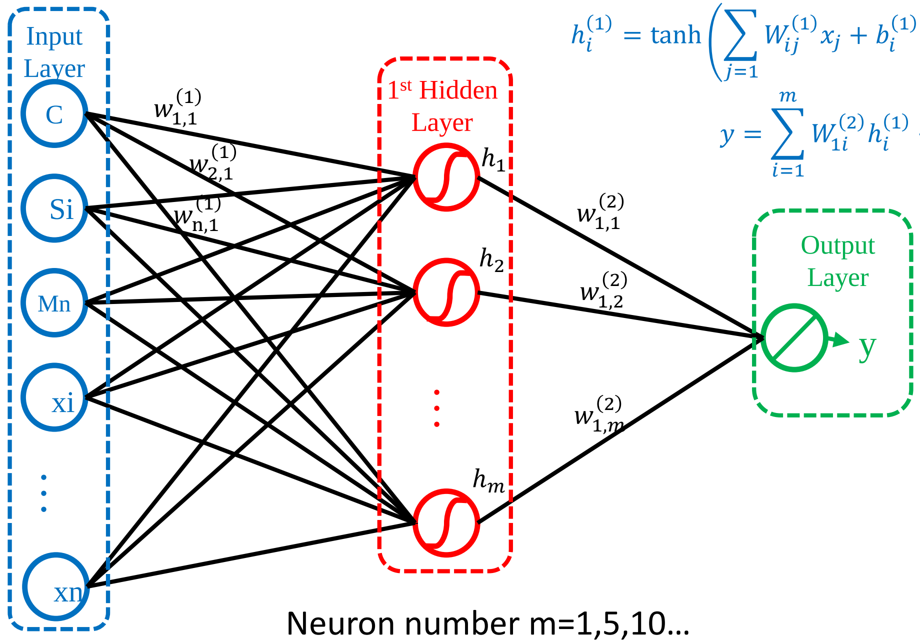
10000+ Real-factory data (excel data sheet)

1 hidden layer shallow neural network

$$h_i^{(1)} = \tanh\left(\sum_{j=1} W_{ij}^{(1)} x_j + b_i^{(1)}\right), i = 1,2,\cdots,n$$

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

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



Output:
Yield strength,
Tensile strength,
Elongation,
σs/σb,
Drop weight tear testing

Neuron number m=1,5,10…

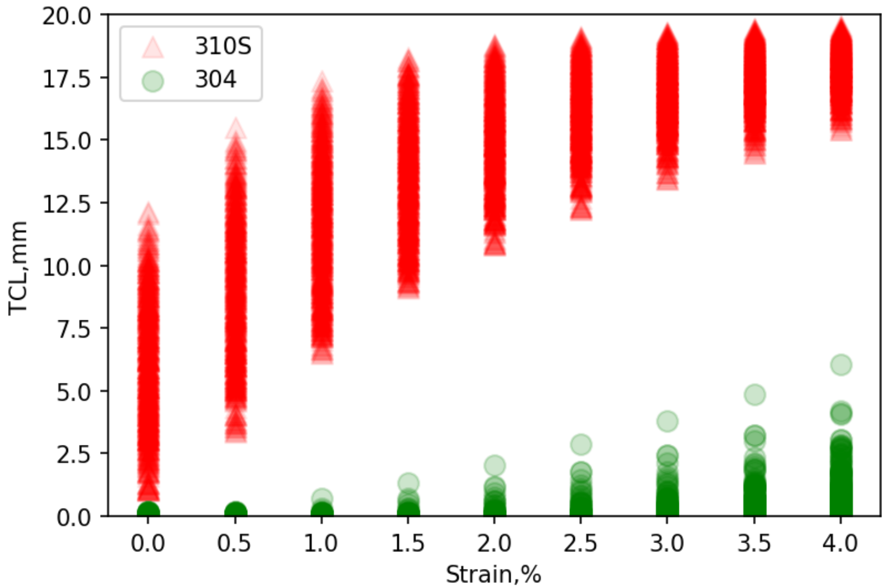
High training & testing accuracy

0.99 (Pearson coefficient of prediction and real data)

Predicting solidification cracking susceptibility of stainless steel

	code	C	Si	Mn	P	S	Cr	Ni	Mo	N	...	V	B	Th	I	U	Ve	Strain	TCL	MCL	note
0	316NG-A	0.0100	0.48	1.61	0.024	0.019	17.33	10.62	2.09	0.0600	...	0.0	0.0	3.18	100	12.0	4.23	4.0	1.50	0.19	ref03
1	316NG-B	0.0110	0.58	1.06	0.032	0.013	16.95	10.50	2.15	0.0780	...	0.0	0.0	3.18	100	12.0	4.23	4.0	1.10	0.18	ref03
2	316NG-C	0.0100	0.46	1.09	0.021	0.001	17.40	11.50	2.88	0.1050	...	0.0	0.0	3.18	100	12.0	4.23	4.0	0.90	0.15	ref03
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...	...
484	K17	0.0140	0.33	1.73	0.026	0.007	17.90	9.50	0.00	0.0460	...	0.0	0.0	5.00	70	16.0	1.25	1.2	0.24	Nan	ref17fig14
485	SUS304	0.0500	0.75	0.94	0.026	0.007	18.30	9.40	0.00	0.0160	...	0.0	0.0	5.00	70	16.0	1.25	1.2	0.00	Nan	ref17fig14
486	SUS316	0.0700	0.66	1.01	0.020	0.006	16.70	12.40	2.38	0.0200	...	0.0	0.0	5.00	70	16.0	1.25	1.2	1.47	Nan	ref17fig14

487 rows × 25 columns



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)

Code	C	Si	Mn	P	S	Cr	Ni	N	Al	Th	I	U	Ve
304	0.06	0.5	1.5	0.005-0.03	0.005-0.03	18-20	8-10.5	0.02	0.02	3.18	100	12	4.23
310S	0.01	0.5	1.5	0.005-0.03	0.005-0.03	24-26	19-22	0.02	0.02	3.18	100	12	4.23

Predicting glass-forming ability

Collect → Process → Represent → Learn → Predict

Dataset size:
10440 entries

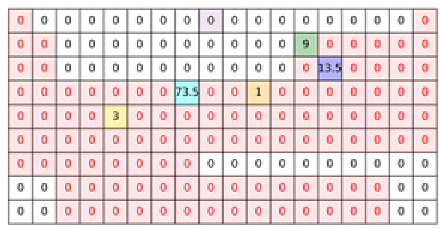
Input: composition
Output: GFA

139: 2 $Al_{32}Ca_{68}$ [Ribbon][44]
140: 2 $Al_{33.6}Ca_{66.4}$ [BMG][38]
141: 2 $Al_{33}Ca_{67}$ [Ribbon][44]
142: 2 $Al_{34}Ca_{66}$ [Ribbon][44]
143: 2 $Al_{35}Ca_{65}$ [Ribbon][44]

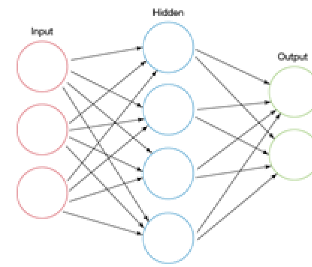
MF: 1-D vector
PTR: 2-D image

$\bar{r}$	$\bar{\chi}$	ΔS_{mix}	ΔH_{mix}	...	c_i

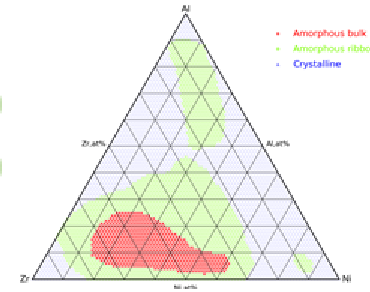
PTR of $Fe_{73.5}Cu_1Nb_3Si_{13.5}B_9$



SNN
CNN



Binary, ternary, etc.



4243: 3 $Al_{52}Fe_{23}Ge_{25}$ [Ribbon][15]
4244: 3 $Al_{69}Fe_{6}Ge_{25}$ [Ribbon][15]
4245: 3 $Al_{78}Fe_{10}Ge_{12}$ [Ribbon][15]
4246: 3 $Al_{25}Fe_{20}La_{55}$ [Ribbon][15]
4247: 3 $Al_{10}Fe_{30}Nd_{60}$ [BMG][16]
4248: 3 $Al_{75}Fe_{14}Ni_{11}$ [Ribbon][15]
4249: 3 $Al_{82}Fe_{4}Ni_{14}$ [None][15]
4250: 3 $Al_{83}Fe_{3}Ni_{14}$ [None][15]
4251: 3 $Al_{84}Fe_{2}Ni_{14}$ [None][15]

10000+ data collected from literature

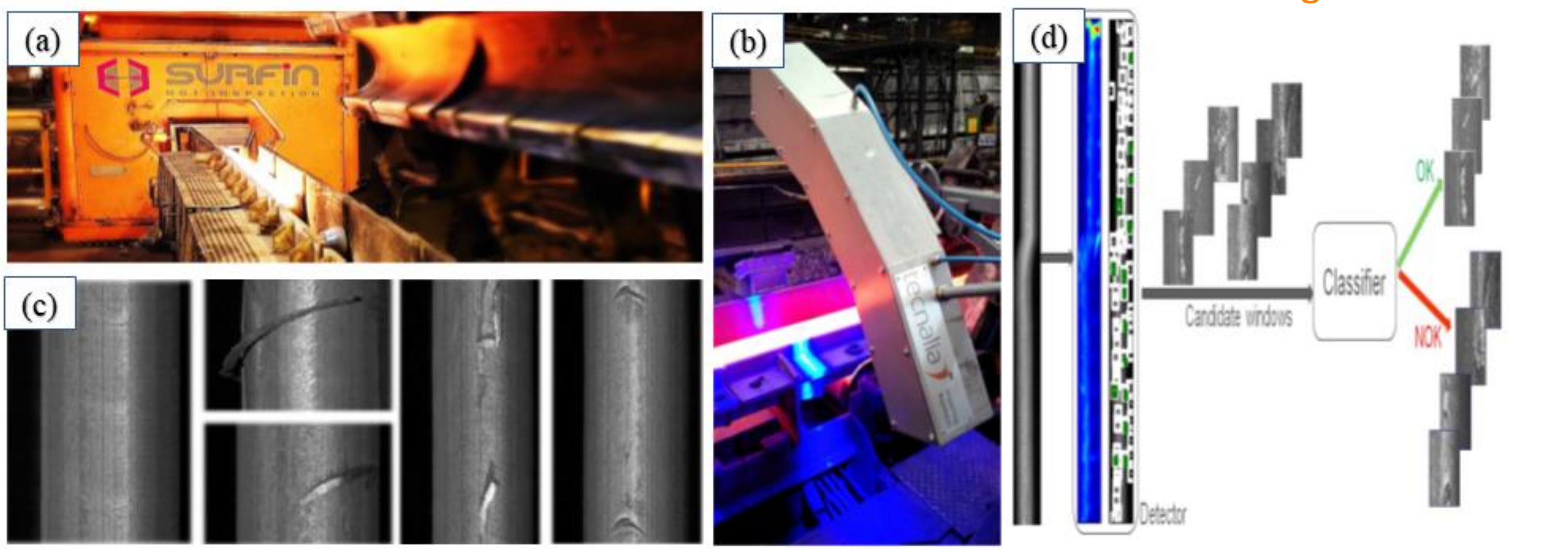
None: not able to form metallic glass
Ribbon: able to form thin (20-30μm) metallic glass
BMG: able to form thick metallic glass (1 mm)

Input: alloy composition

3 labels: None, Ribbon, BMG

Defect detection

Image classification



Online, high speed (>10m/s), high temperature (>1000 ℃) metal products' surface quality inspection

	# images		Defect type
OK	2475		
NOK	1411	315	Roll Mark
		887	Folds
		209	Cracks
TOTAL	3886		

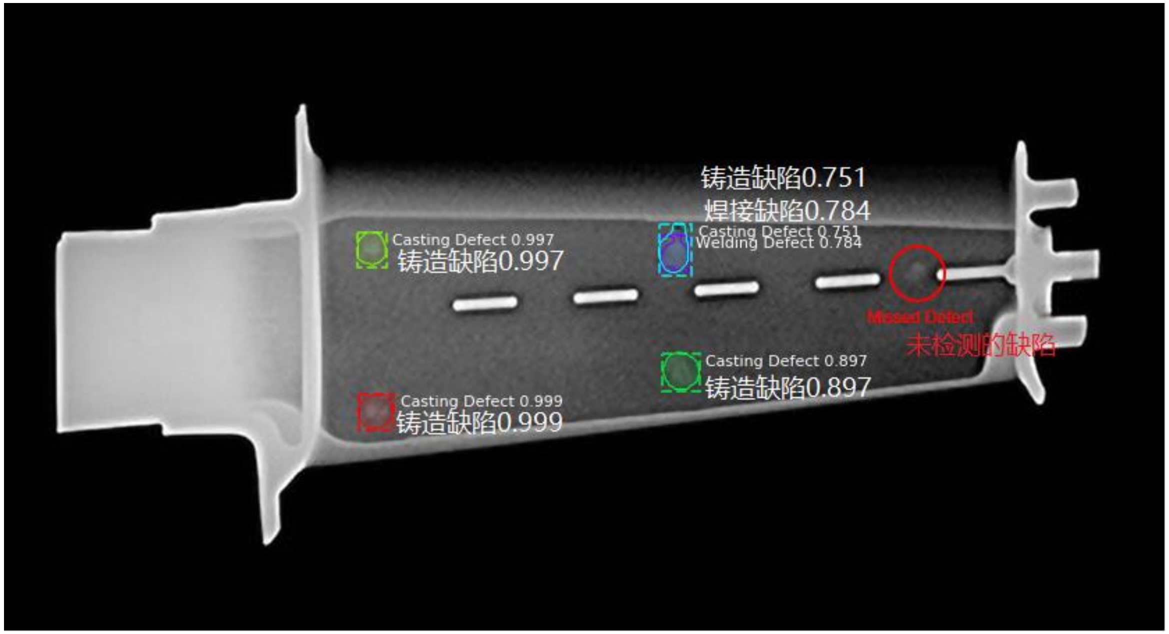
2-class classification (OK vs. NOK)

Feature extraction	Classifier	AUC
Commercial	Commercial (SVM)	0.88
LBP features	SVM	0.92
LBP features	Random Forests	0.95
CNN-SURFIN (feature extractor + classifier)		**0.997**

[1] https://computervision.tecnalia.com/en/

Defect detection

Object detection



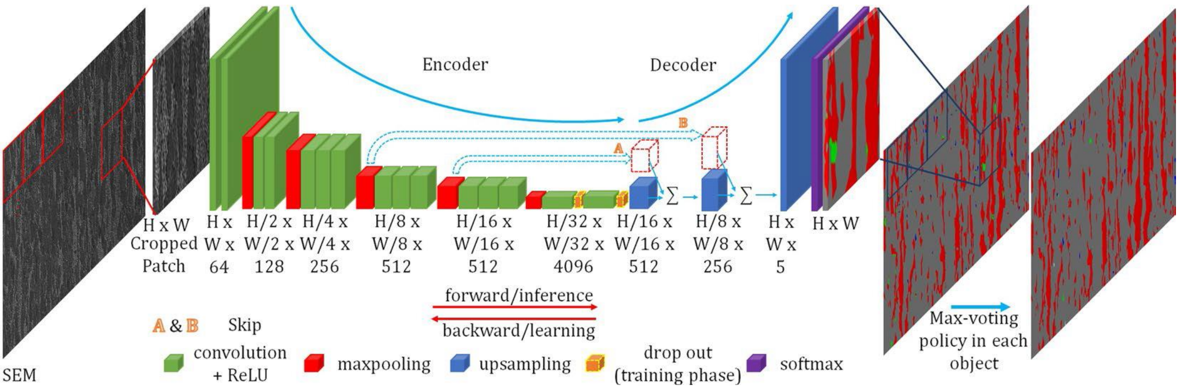
Defect detection on an X-ray image of a jet turbine blade

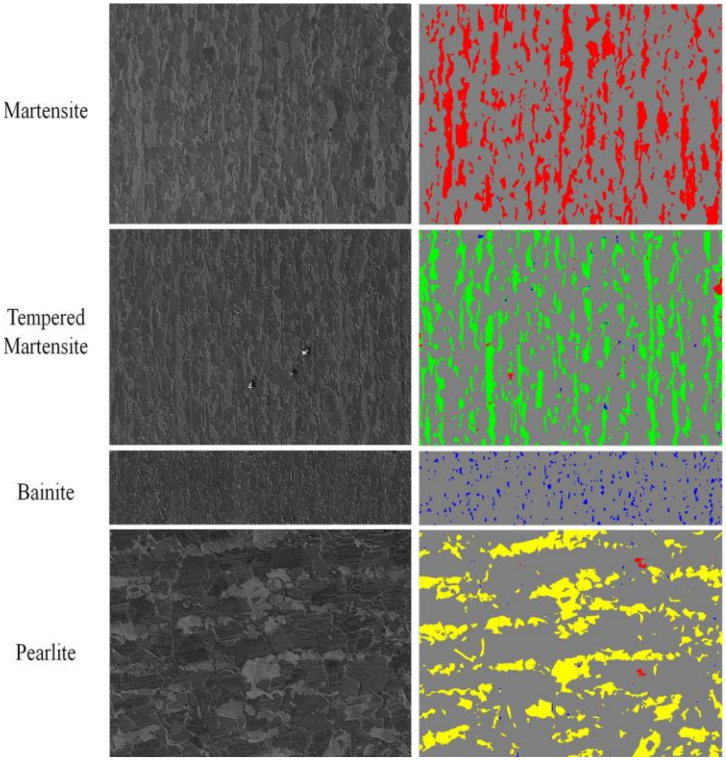
The training dataset did not contain any turbine blade images.

[1] FERGUSON M, AK R, LEE Y-T T, et al. 2018. Detection and Segmentation of Manufacturing Defects with Convolutional Neural Networks and Transfer Learning. arXiv preprint arXiv:1808.02518 [J].

Microstructure recognition

Image segmentation





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

[1] AZIMI S M, BRITZ D, ENGSTLER M, et al. 2018. Advanced Steel Microstructural Classification by Deep Learning Methods. Scientific reports [J], 8: 2128.

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

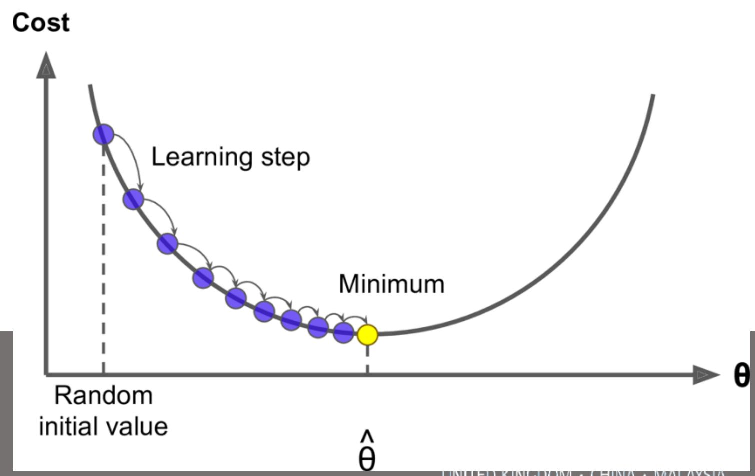
To improve generalization, add msw (mean square weight) to simple loss function J(θ) e.g. mse (mean square error)

$$\boxed{\mathrm{mse}} = \frac{1}{N}\sum_{i=1}^{N}(e_i)^2 = \frac{1}{N}\sum_{i=1}^{N}(t_i - a_i)^2 \qquad \boxed{\mathrm{msw}} = \frac{1}{n}\sum_{j=1}^{n} w_j^2$$

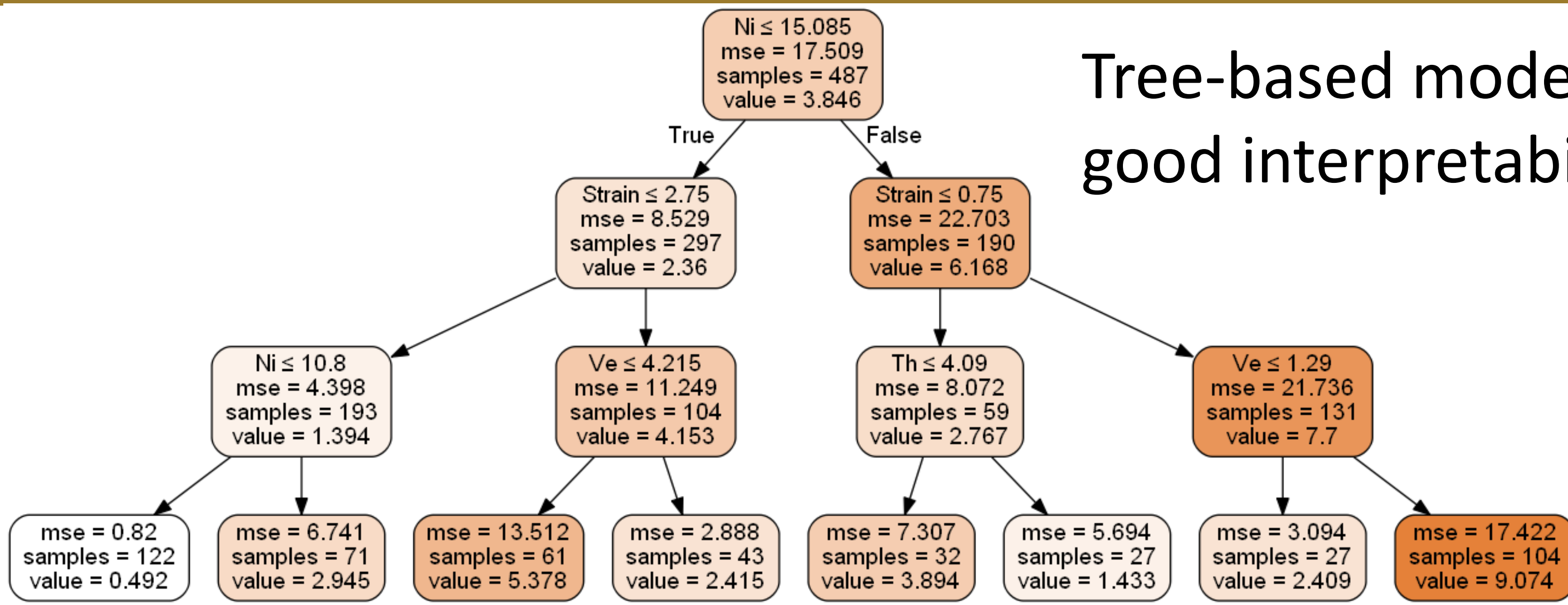
$$\mathbf{J(\theta)} = \mathrm{msereg} = \gamma\,\mathrm{mse} + (1-\gamma)\,\mathrm{msw}$$

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

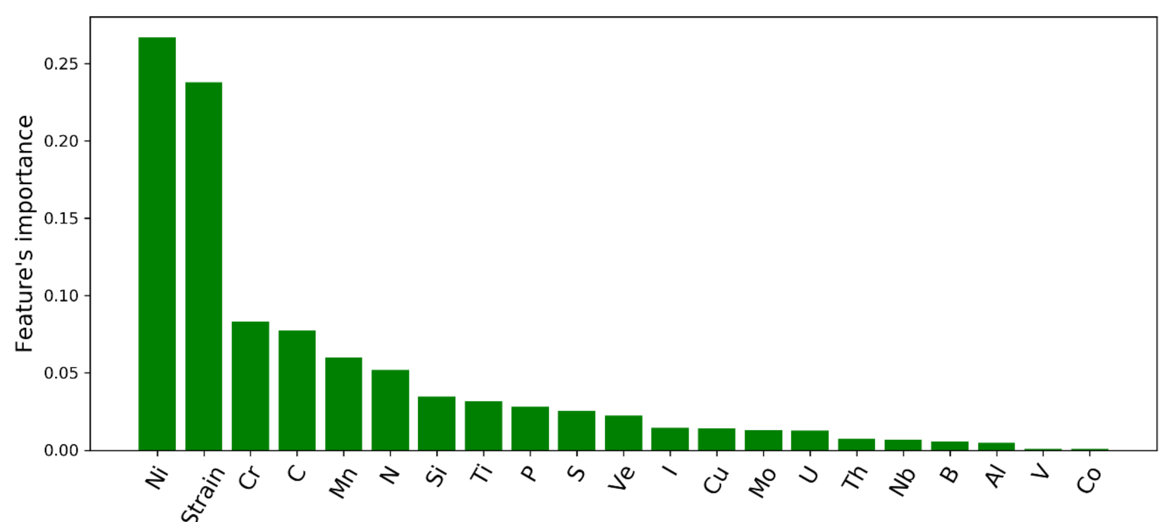
Backpropagation algorithm



Black box models ?



Tree-based models: good interpretability



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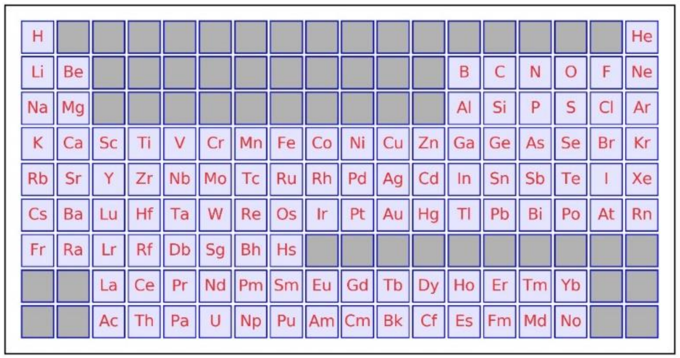
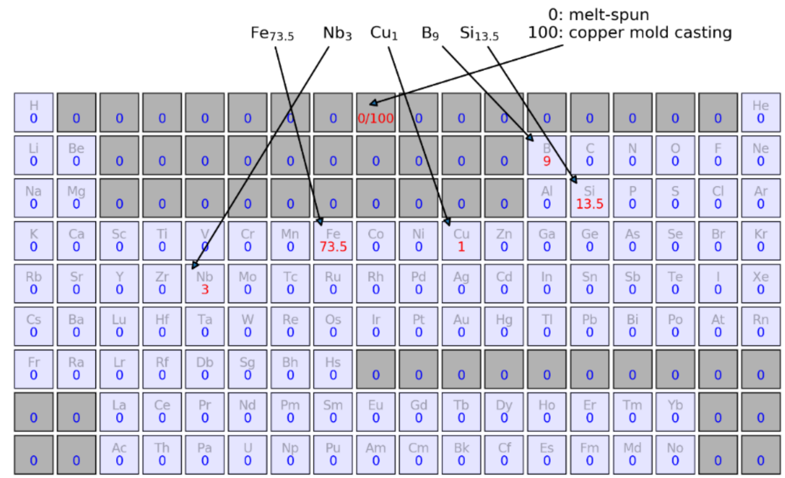
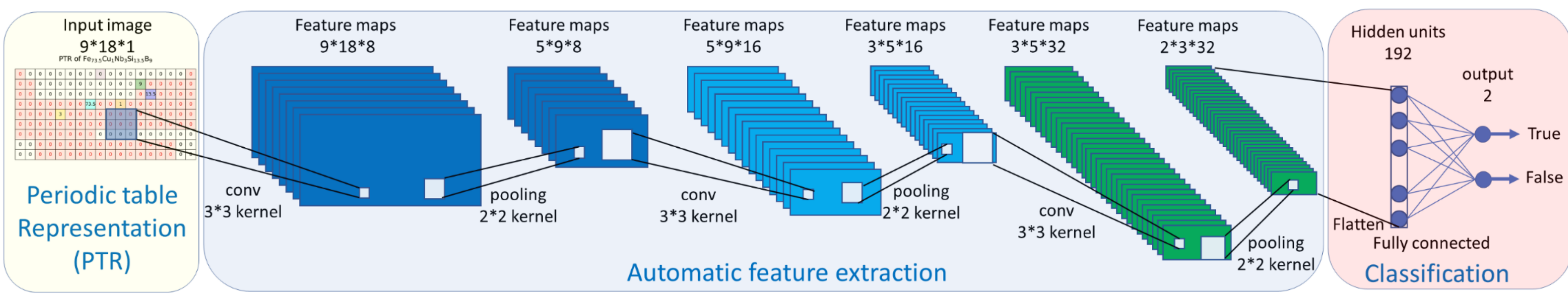
Exploit deep learning

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





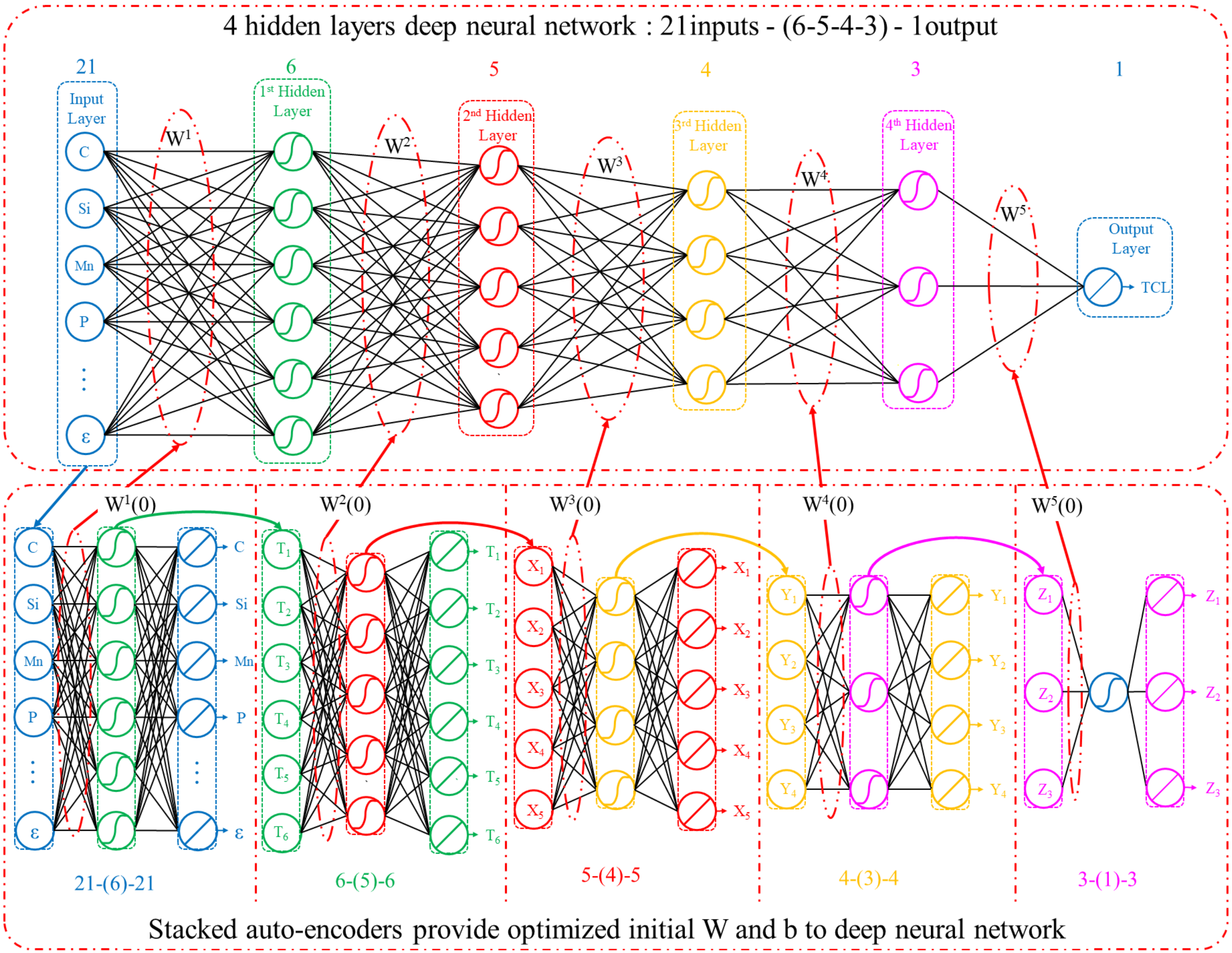


Only composition is needed to predict glass-forming ability

Input → 3*3/Conv/8 filter →max pooling → 3*3/Conv/16 filter → max pooling → 3*3/Conv/32 filter → max pooling → flatten → FC → **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)

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!

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