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Machine learning for resonant ultrasound spectroscopy of isotropic materials

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Non-destructive testing and evaluation

- **Purpose:** Evaluate the integrity of materials, determine physical properties of components, or systems without causing any damage
- **Need:** Crucial for ensuring the safety and reliability of critical structures in industries
- **Methods**: Thermography, ultrasound, eddy current, radiography, microwave, and hybrid methods
- **Mode**: Analysis of time or frequency domain signals, images, or videos

Medical testing

Electrical inspection

Concrete pipe inspection

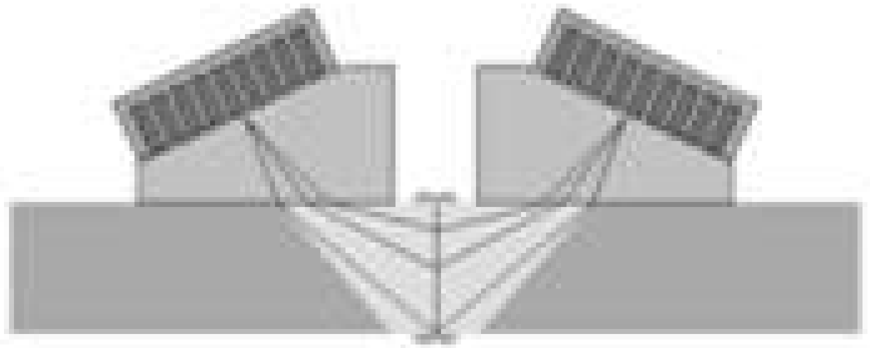
Material inspection

Ultrasonic Non-destructive Evaluation

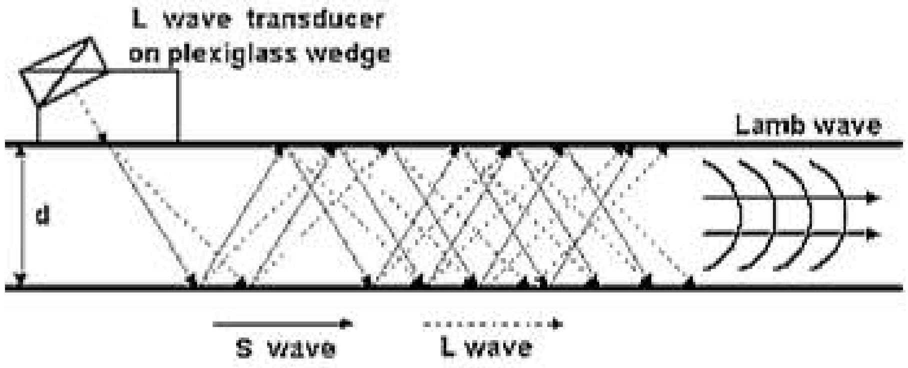
- **Ultrasonics:** Use sound waves of frequencies > 20 kHz
- **Working principle:** A transducer generates ultrasonic waves that travel through the material and reflect back from discontinuities, such as cracks or inclusions, which are then captured and analysed and estimated elastic constants.
- Non-invasive and safe for both the operator and the material being tested

Methods in Ultrasound testing

Time of flight diffraction (ToFD)



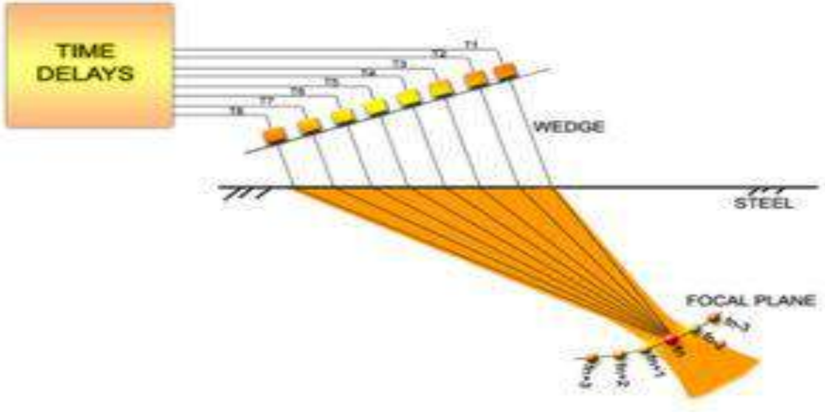
Guided wave testing



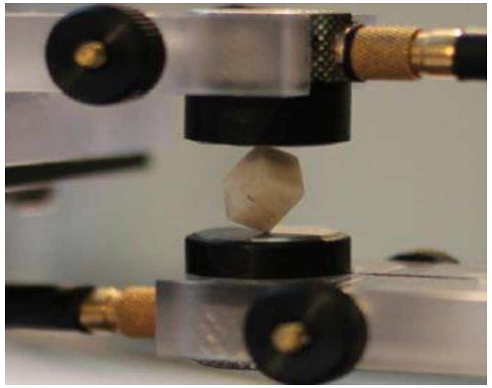
https://www.youtube.com/watch?app=desktop&v=UM6XKvXWVFA

Methods in Ultrasound testing

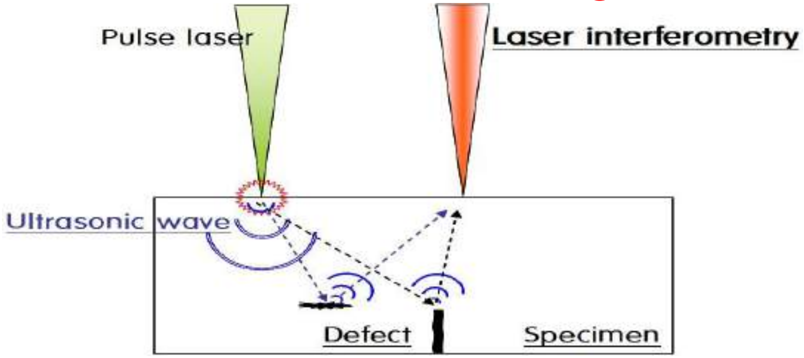
Phased array ultrasonics



Resonant ultrasound spectroscopy (RUS)



Laser ultrasonics testing



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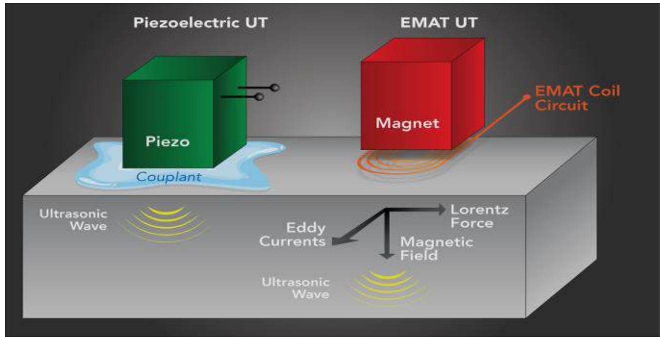


- Among all these more preferably ToFD and guided ways are used for estimating elastic constants.
- RUS does the same but it is more delicate and easy to implement for determining elastic constants.

What are elastic constants?

Properties of material that describe the relation between stress and strain

Constitutive relation: Tensor form

$$\underline{\sigma} = \underline{\underline{\underline{C}}}\,\underline{\epsilon}$$

Voigt form

$$\underline{\sigma}_{6\times1} = \underline{\underline{C}}_{6\times6}\,\underline{\epsilon}_{6\times1}$$

Matrix form

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

$\underline{\underline{C}}_{6\times6}$ - Stiffness or elastic matrix (Symmetric). Maximum of 21 independent constants

Isotropic materials

Isotropic materials have identical properties in all directions and two independent elastic constants.

Constitutive relation:

Tensor form -

$$\underline{\underline{\sigma}} = \lambda \, \mathrm{tr} \underline{\underline{\epsilon}} \, \mathbf{I} + 2\mu \, \underline{\underline{\epsilon}}$$

Matrix form -

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} 2\mu + \lambda & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & 2\mu + \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & 2\mu + \lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

λ and μ are the Lame's parameters and are related to the Young's modulus $\boldsymbol{E}$ and Poisson's ratio $\boldsymbol{\nu}$.

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)} \qquad \mu = \frac{E}{2(1+\nu)}$$

Importance of elastic constants

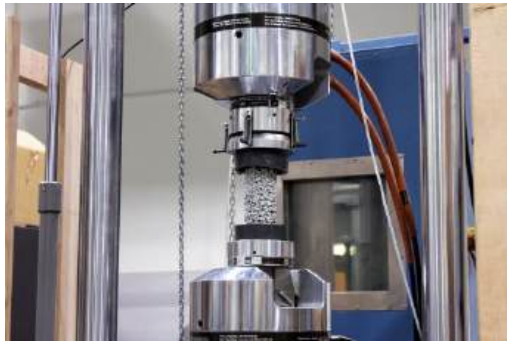
- To design safe and efficient structures
- Predicting and preventing material failure
- Development of reliable and durable system

Need to elastic constants

- Evaluating the existing structure and defining its life
- Estimating flaws and maintaining the standard of material
- Predict behaviour of material accurately
- Precise calculation for engineering design

Ways of measuring elastic constants

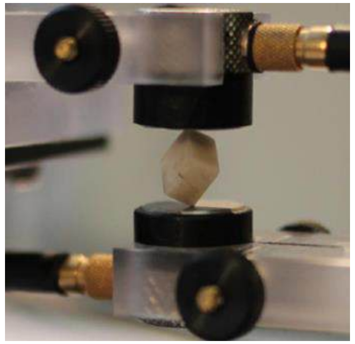
Tensile testing



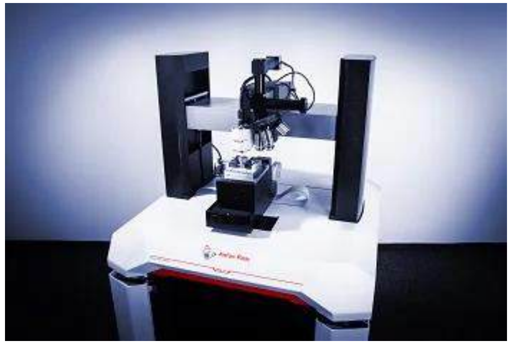
Compression testing

Flexural testing

Brillouin Scattering



RUS



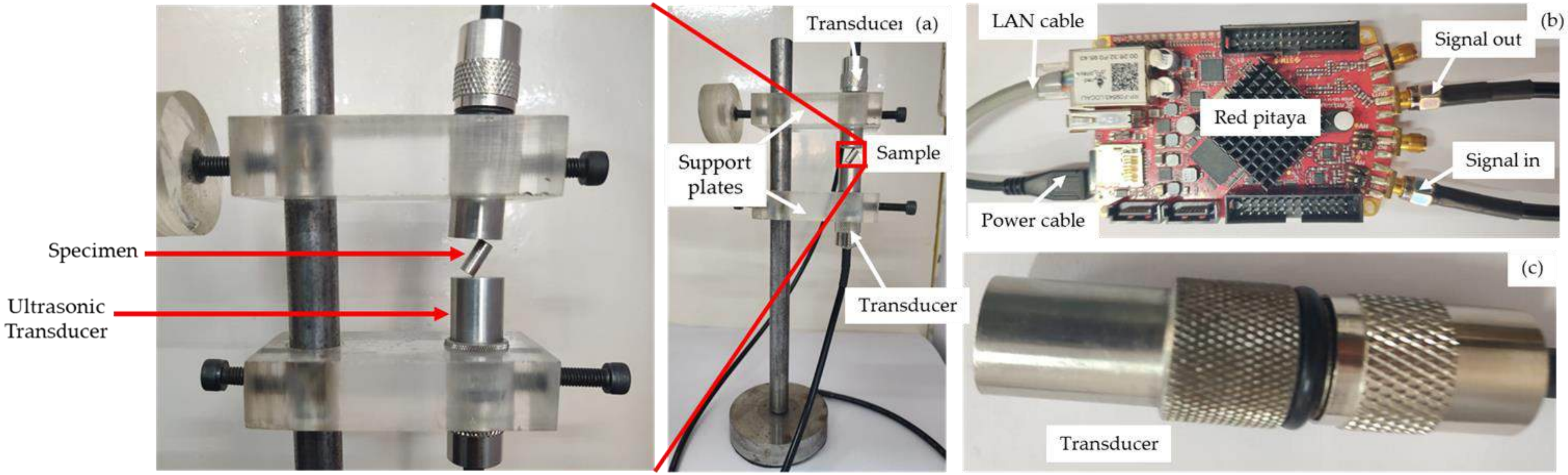
Nanoindentation

Ultrasound testing

Dynamic mechanical analysis

Resonant Ultrasound Spectroscopy

- A dedicated non-destructive technique to measure the elastic constants by analyzing their resonant frequencies



- A sample is excited using an ultrasonic transducer, causing it to vibrate at its resonant frequencies
- Frequencies are then calculated and an optimization problem is solved to determine $\underline{\underline{C}}_{6\times 6}$

Theory of an RUS experiment

Kinematics $\underline{\epsilon} = D_\epsilon u$

$$D_\epsilon = \begin{bmatrix} \partial/\partial x & 0 & 0 \\ 0 & \partial/\partial y & 0 \\ 0 & 0 & \partial/\partial z \\ 0 & \partial/\partial z & \partial/\partial y \\ \partial/\partial z & 0 & \partial/\partial x \\ \partial/\partial y & \partial/\partial x & 0 \end{bmatrix}$$

Constitutive relation $\underline{\sigma} = C\underline{\epsilon} = CD_\epsilon u$

Force balance $D_\epsilon^T \sigma + b = -\rho\omega^2 u$

Governing equations $D_\epsilon^T C D_\epsilon u + b = -\rho\omega^2 u$

- This is also called Christoffel equation
- The specimen is considered traction-free on its entire boundary

Numerical intricacies in RUS analysis

- Levenberg-Marquardt algorithm is used to fit the measured resonant frequencies to the Christoffel equation. , adjusting elastic constants and solves nonlinear least square problem.
- Objective function: $$\chi^2(X) = \sum_i \left(f_i^{\text{measured}} - f_i^{\text{theoretical}}(X)\right)^2$$
- This algorithm updates elastic constants *C* iteratively using

$$X_{k+1} = X_k - (J_k^T J_k + \lambda_k I)^{-1} J_k^T r_k$$

where, $X = \begin{bmatrix} E & \nu \end{bmatrix}$

λ - Damping parameter

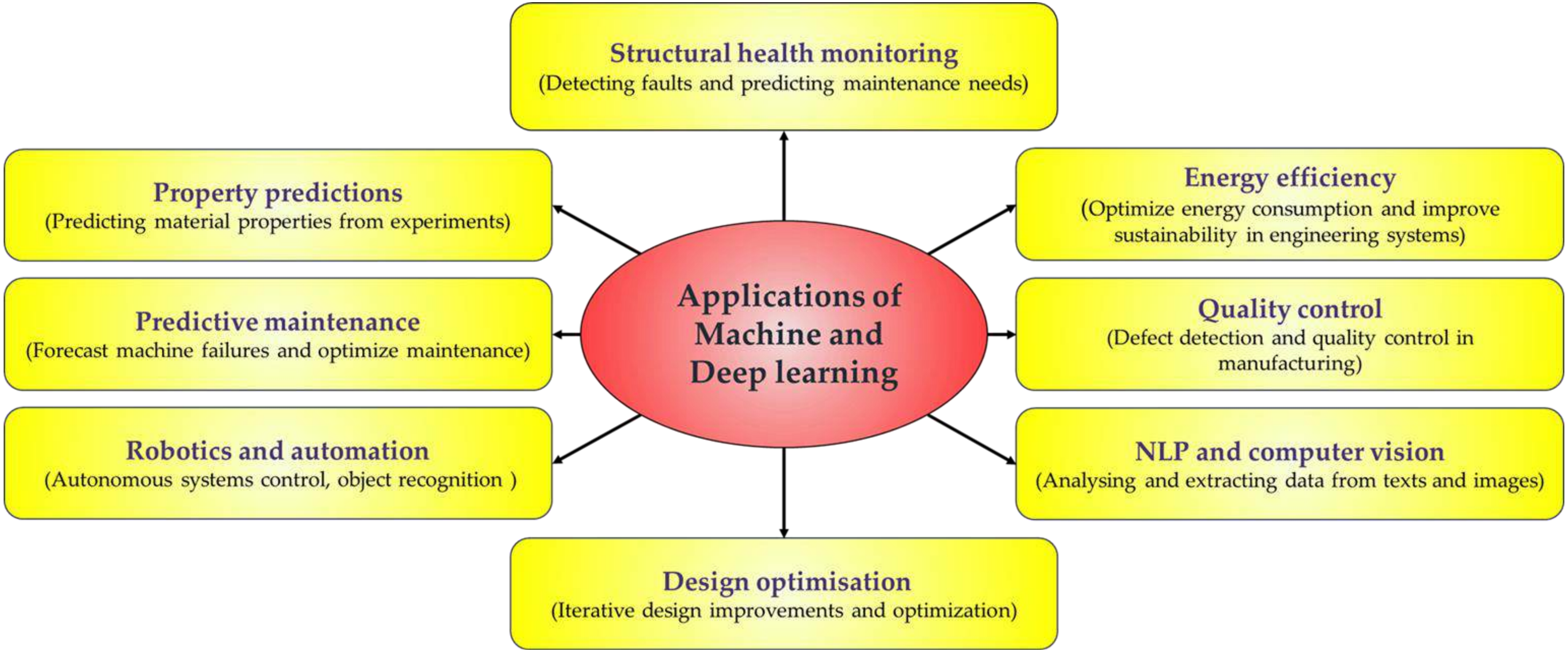
I - Identity matrix

r - Residual vecto $(r = f_{\text{measured}} - f_{\text{theoretical}}(X))$

J - Jacobian matrix, $J_{ij} = \dfrac{\partial f_{\text{theoretical},i}}{\partial X_j}$

Machine and deep learning models

Revolutionizing engineering and technology by enabling computers to learn from data, uncover patterns, and make intelligent decisions, paving the way for unprecedented innovation and efficiency.



Our approach

Excite the specimen using ultrasonic transducers

Acquire response and identify the eigenfrequencies

Traditional method

Fit the acquired eigenfrequencies to a theoretical model using the Levenberg-Marquardt algorithm

Limitations

- Computation time for materials with higher symmetries is in hours & days
- Insensible to noisy input

Our approach

Fit the acquired eigenfrequencies along with density and size of specimen to a trained ML & DL models

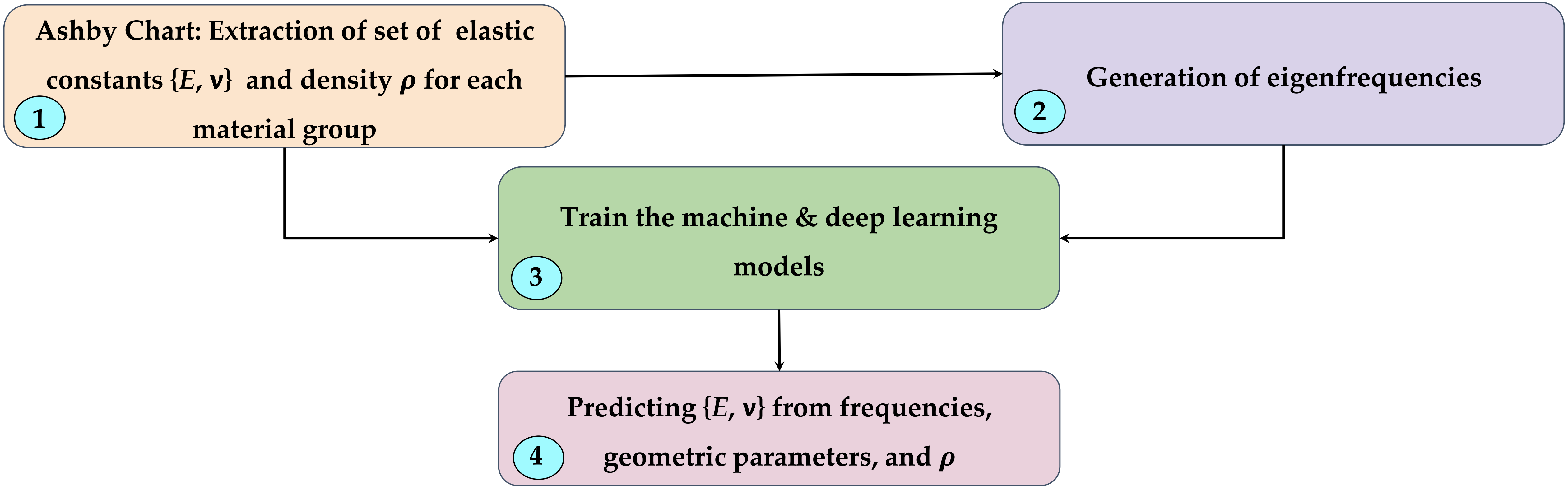
Advantages

- Orders faster than traditional methods
- Make onsite decisions in seconds.
- ML solutions can also assist with inverse problems by providing initial guesses

Determine the elastic constants

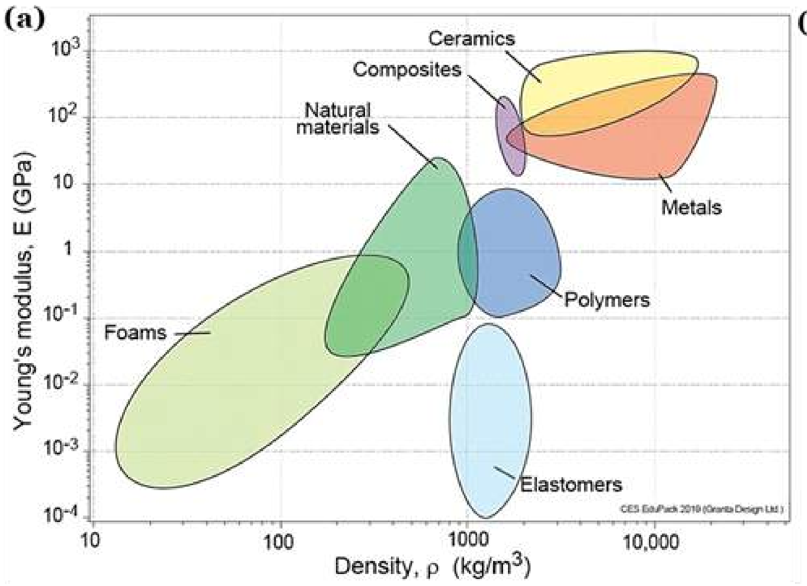
Framework overview

- **First attempt of ML in RUS:** Focus exclusively on isotropic materials
- **Standard shapes used in RUS:** Cuboid {a, b, c} and cylinder {l, r}
- **Material classes considered:** Metals and alloys, ceramics, polymers



1 Extraction of data from Ashby chart

- The process of generating random set of $\{\boldsymbol{\rho}, E, \boldsymbol{\nu}\}$ is:



(b)

Upload image of E vs ρ Ashby chart in WebplotDigitizer

↓

Define the coordinate axes and chose the plot type

↓

Select maximum number of points on the boundary for every class of materials and import them as a CSV file

↓

Generate a uniform distribution of (ρ, E) within the boundary using Python

↓

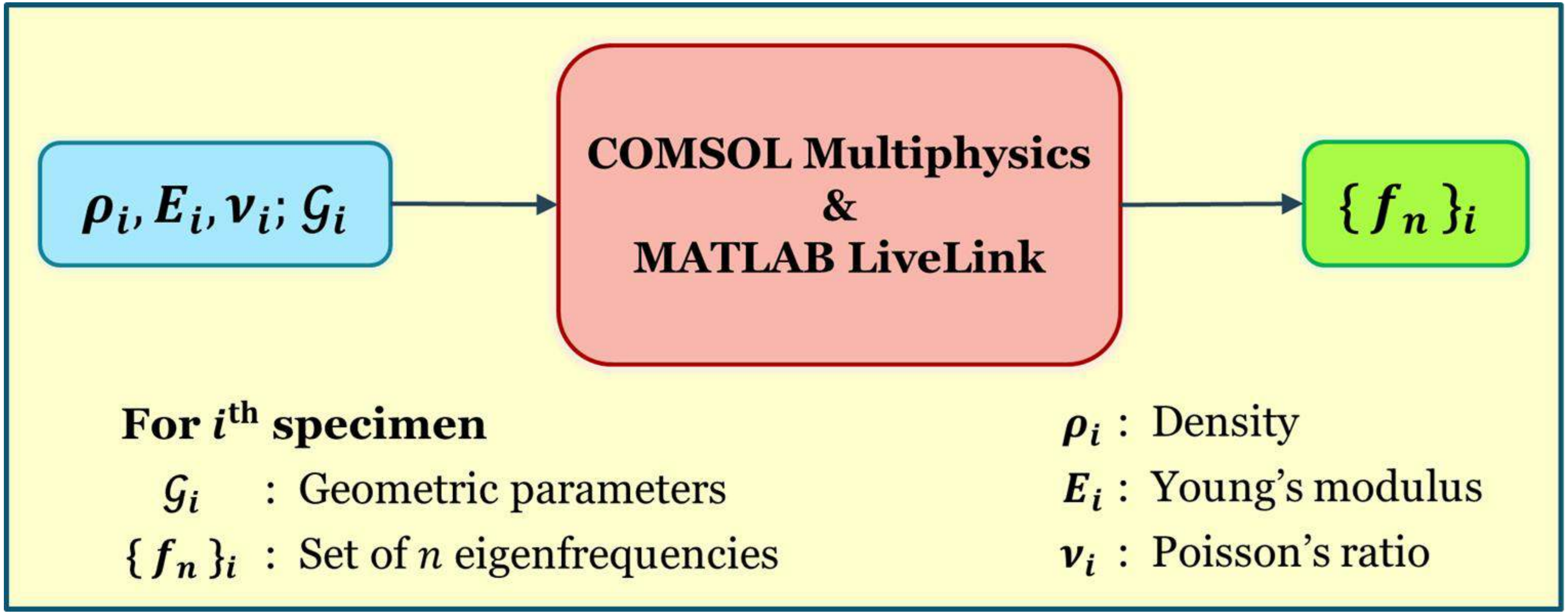
Generate random sets of (ρ, E, ν) using uniform distribution

Identify the range of ν for every class of materials from at least 200 materials → Generate random sets of (ρ, E, ν) using uniform distribution

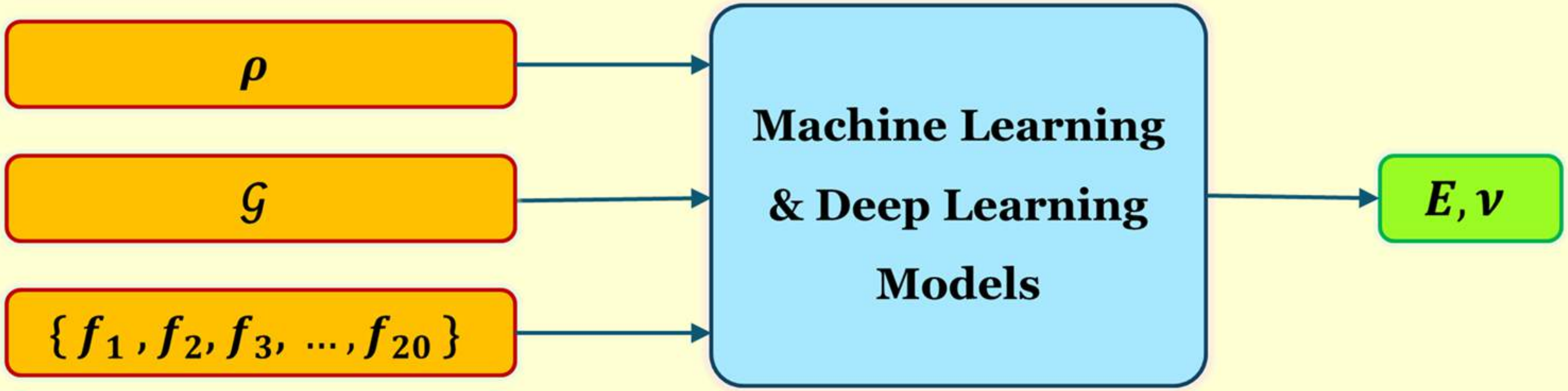
(a) Ashby chart and (b) Flowchart of data extraction from Ashby chart

2 Generation of eigenfrequency for training

- Generated eigenfrequencies for each material group (metals, ceramics, & polymers) and each shape (cuboidal and cylindrical)



3 Machine learning and deep learning models and their training

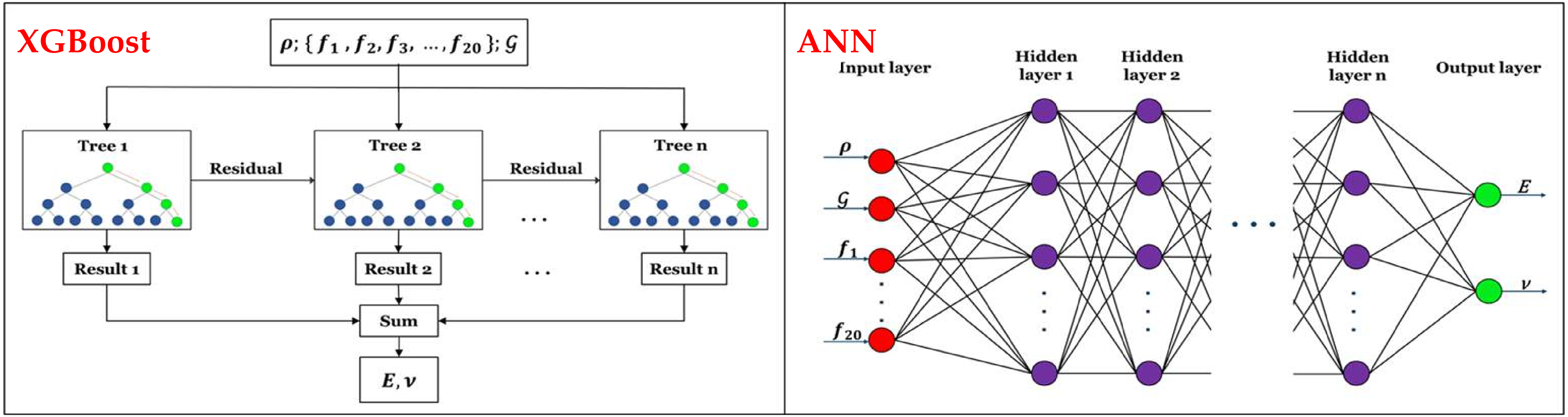


Machine learning models : Random forest, XGBoost
Deep learning models : ANN

- For cylinder shape each material group consists of 1,50,000 datasets and for cuboid 2,40,000 datasets.

Overview of machine learning and deep learning algorithms

- **XGBoost** : An advanced gradient boosting algorithm that builds an ensemble of decision trees to enhance predictive accuracy and efficiency
- **ANN** : Mimics the network (interconnected nodes organized in hidden layers) and working (mirroring the learning process) of the human brain

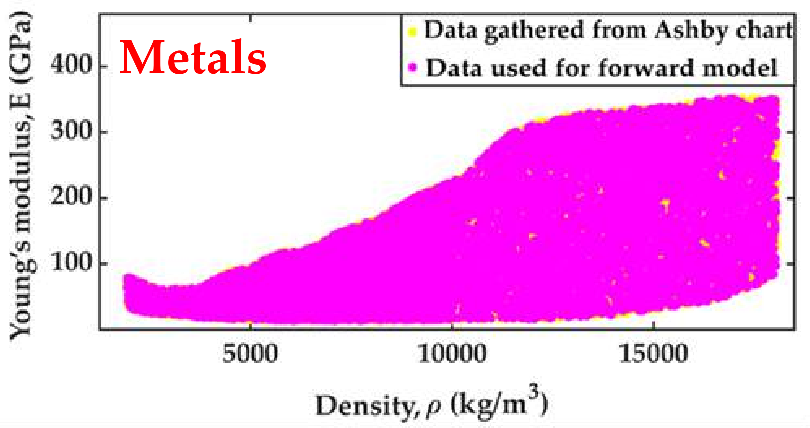


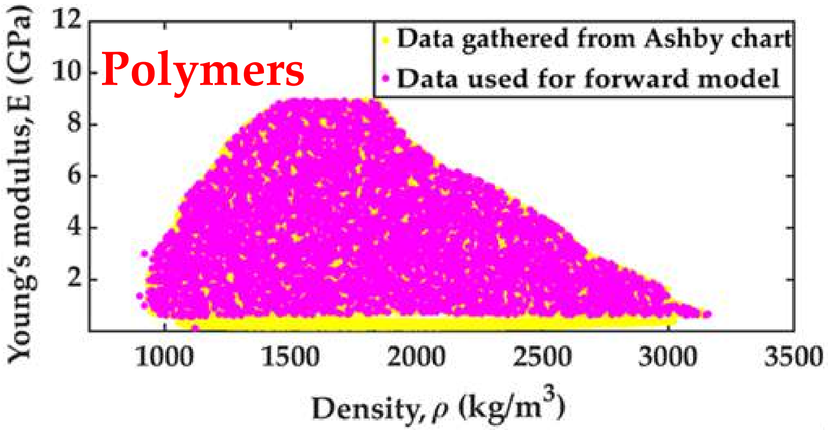
Model tuning and training details

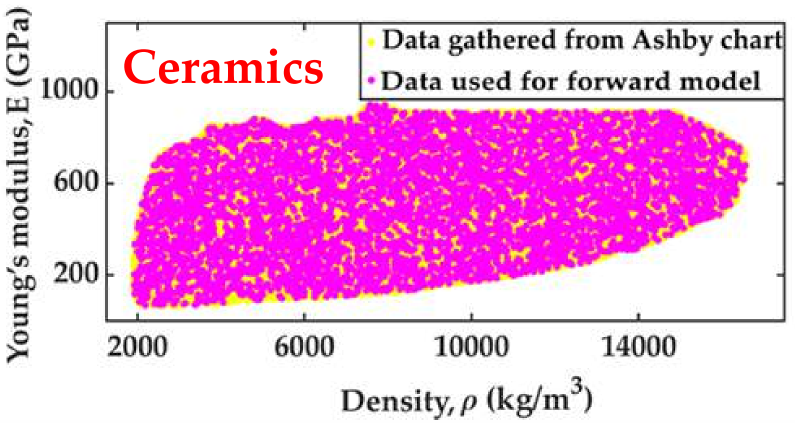
	Learning rate	Estimators	Epochs	Hidden layers	Rest parameters as default
XGBoost	0.00001 to 0.3	5000 to 75000	-	-	
ANN	0.00001 to 0.3	-	500 to 2000	3 to 7	

- ANN model: 6 hidden layers with number of neurons as 128, 64, 32, 16, 8 and 4.
- 1% of datasets were used for testing; remaining for training
- Model trained with three different approaches scaling to order 10^3:
  - Without scaled
  - Only **ν** scaled
  - Both *E* and **ν** scaled

Results from data extraction using Ashby chart







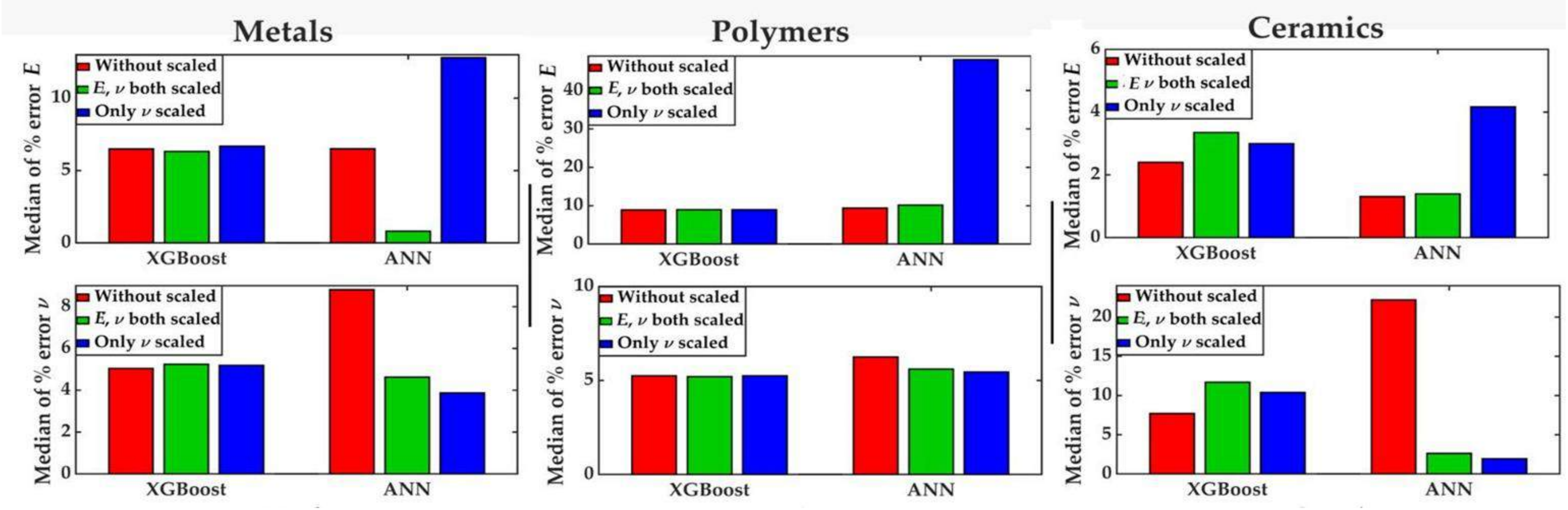
Maximum and minimum of material properties

Material properties	Density (kg/m^3)		Young's modulus (GPa)		Poisson's ratio	
Material class	Min.	Max.	Min.	Max.	Min.	Max.
Metals and alloys	1940.75	18044.69	13.89	351.61	0.23	0.36
Polymers	934.90	3158.07	0.16	8.92	0.36	0.49
Ceramics	1891.63	16563.09	66.16	942.56	0.15	0.48

Analysis of model hyper parameters

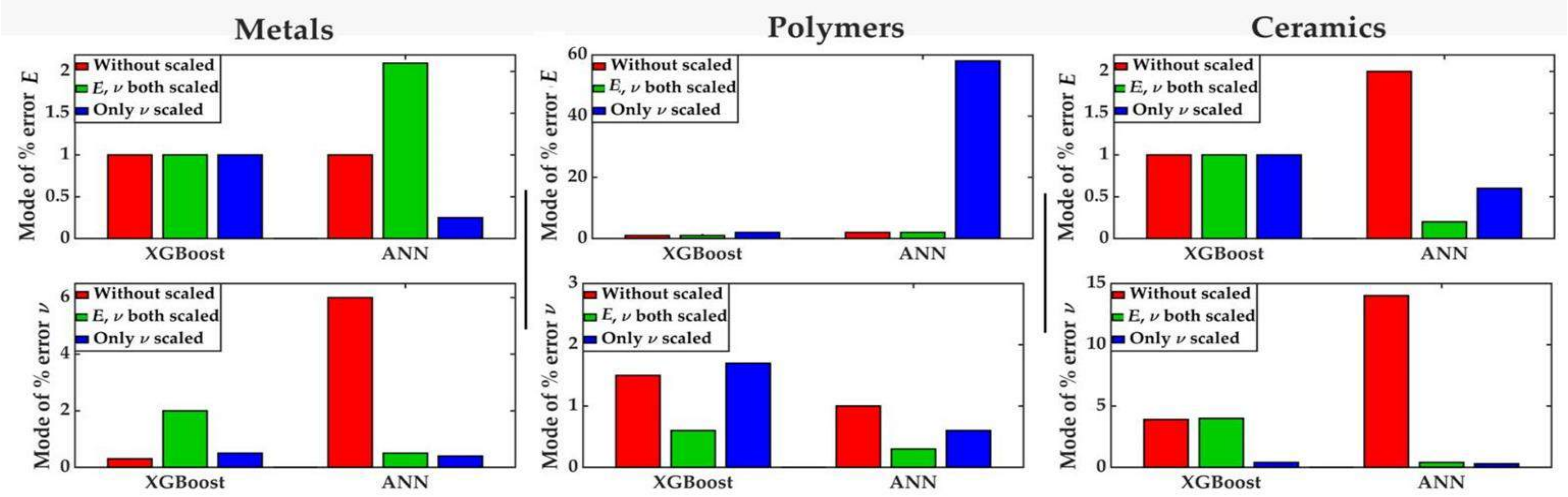
Material class	ML and DL models	Learning rate		Estimators		Epochs	
		Cylinder	Cuboid	Cylinder	Cuboid	Cylinder	Cuboid
Metals and alloys	XGBoost	0.003	0.004	80000	100000	-	-
	ANN	0.0001	0.0003	-	-	1000	1500
Polymers	XGBoost	0.003	0.004	100000	150000	-	-
	ANN	0.0001	0.0001	-	-	1500	1000
Ceramics	XGBoost	0.001	0.003	80000	150000	-	-
	ANN	0.0001	0.0001	-	-	1500	1500

Median percentage error in prediction of elastic constants for cylinders



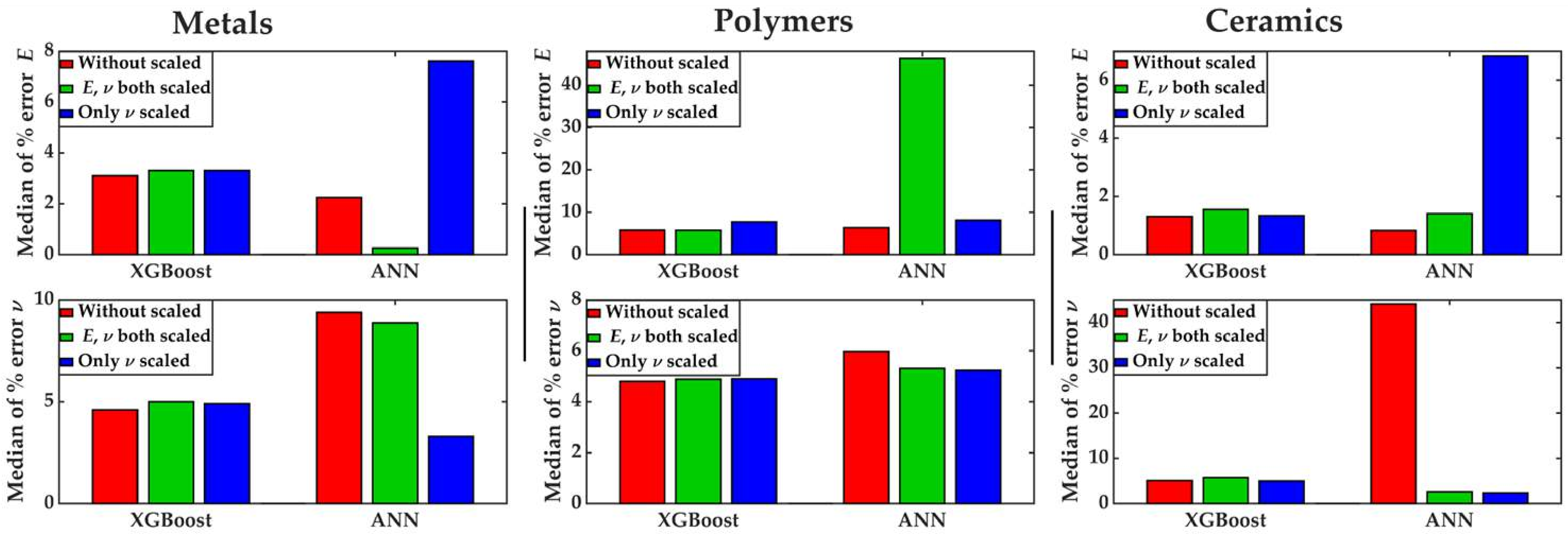
Conclusion: Scaling of E and ν significantly enhances predictive accuracy for XGBoost and ANN models across metals, polymers, and ceramics

Mode of percentage error in prediction of elastic constants for cylinders



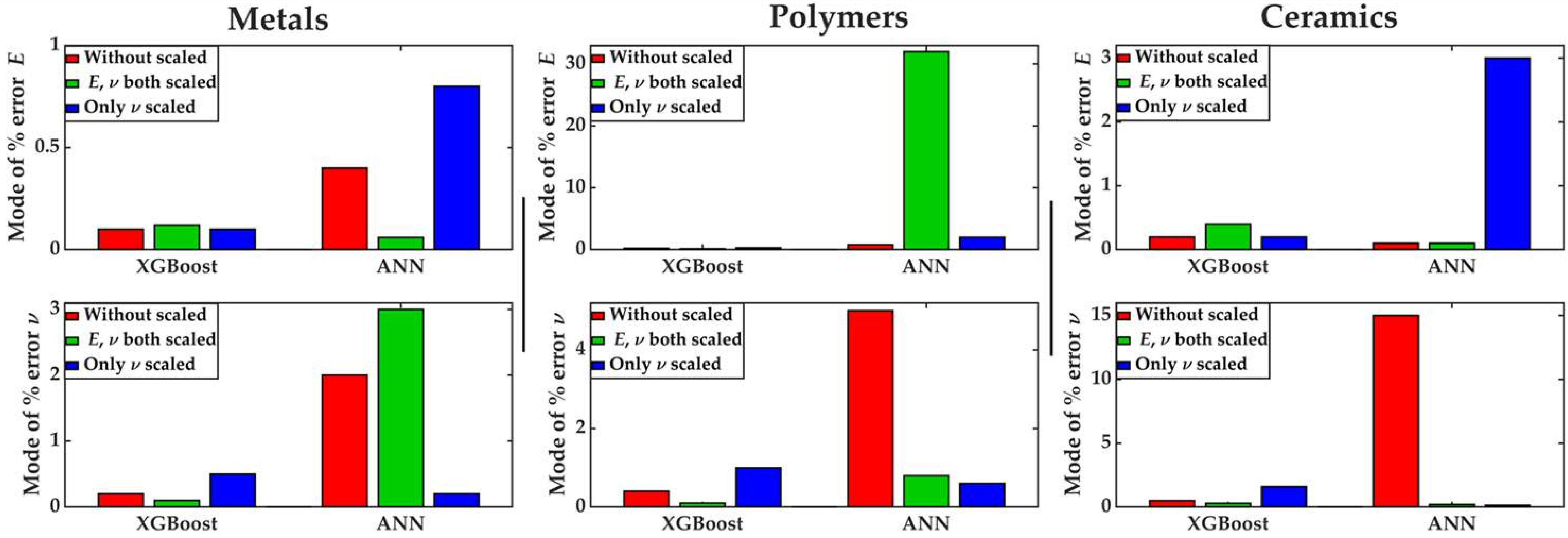
Conclusion: XGBoost almost shows constant trend, but scaling improved the predictions.

Median percentage error in prediction of elastic constants for cuboids



Conclusion: XGBoost almost shows a constant trend, but ANN gave better result upon scaling.

Mode of percentage error in prediction of elastic constants for cuboids



Conclusion: Except for polymers with scaling ANN have some good results and sometimes without scaling

ML/ DL best models in prediction of elastic constants with lower error

Cylinders

Materials	Young's modulus			Poisson's ratio		
	ML\DL Model	Median of % error	MAPE	ML\DL Model	Median of % error	MAPE
Metals	ANN scaled	0.8	4.6	ANN scaled	3.9	6.1
Polymers	XGBoost without scaled	8.9	12.3	XGBoost without scaled	5.2	5.4
Ceramics	ANN without scaled	1.3	3.3	ANN scaled	1.9	6.8

Cuboids

Materials	Young's modulus			Poisson's ratio		
	ML\DL Model	Median of % error	MAPE	ML\DL Model	Median of % error	MAPE
Metals	ANN scaled	0.26	0.46	ANN ν scaled	3.30	5.48
Polymers	XGBoost ν scaled	5.76	9.23	XGBoost without scaled	4.79	5.62
Ceramics	ANN without scaled	0.83	1.74	ANN ν scaled	2.38	5.61

Conclusions

- Developed dedicated ML and DL models for each material class and shape
  - ➢ Used Ashby chart and generated dataset using COMSOL and MATLAB LiveLink
- Demonstrated efficacy of ML, particularly ANN and XGBoost models
  - ➢ Accurately predicted E and ν with median % errors of less than 5% for almost all materials
  - ➢ Exceptions noted for polymers due to their wide range of Young's modulus
- Future work
  - ➢ Expand dataset to include a broader range of shapes and material symmetries
  - ➢ Continuous refinement and expansion of methodologies expected to enhance predictive accuracy and applicability.

Authors contributions

- KPS did all the calculations with the supervision of CC, who also planned the project.
- The presentation was done jointly.

Acknowledgements

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Thank You