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multiphysique, multiéchelle

Contribution of Micromechanics and Machine-Learning to multi-scale modeling of heterogeneous materials

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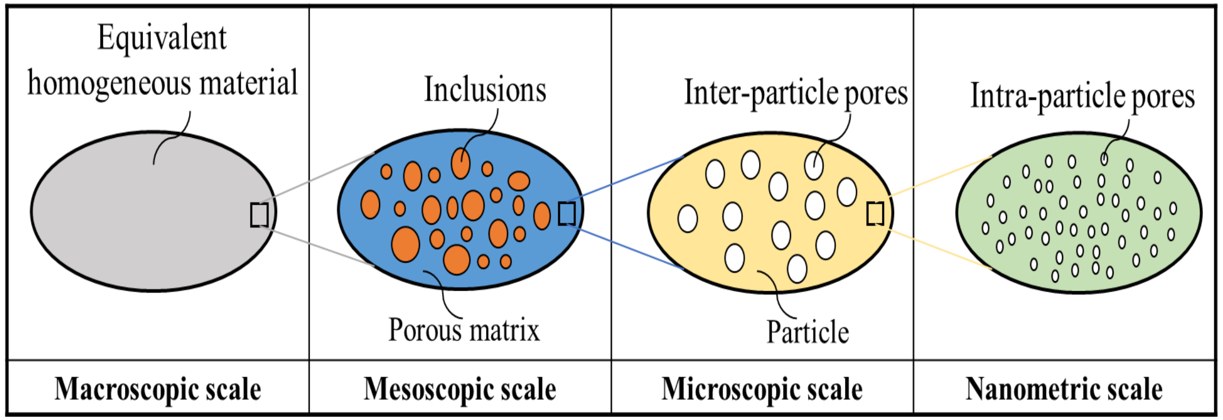
1. Background and motivation



Micro-structures ↔ **Macroscopic properties**

Analytical homogenization methods; simplification of microstructure

Machine-learning based methods; dataset construction

Numerical upscaling methods; high computing cost

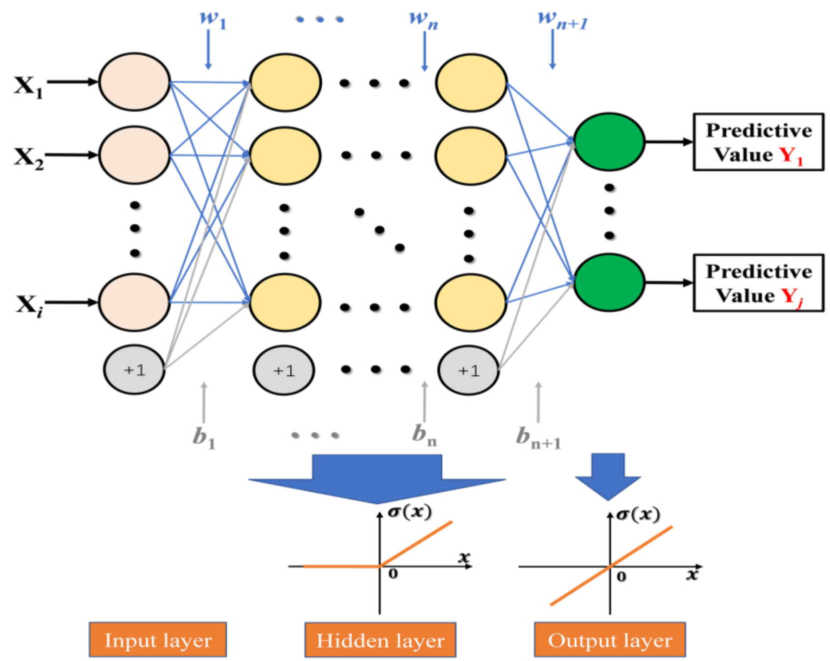
1. Background and motivation

➢ Three key issues:

- ✓ **Identification of constituents properties**
  - ○ **Direct microscopic tests, not always possible, expansive**
  - ○ **ML solutions, macro to micro, use of conventional data such as R_c and R_t**
- ✓ **Prediction of macroscopic properties and their uncertainty**
  - ○ **Analytical micromechanical models, simplified RVE**
  - ○ **Stochastic ML models, complex microstructures**
- ✓ **Improvement of materials performance (3D printing)**

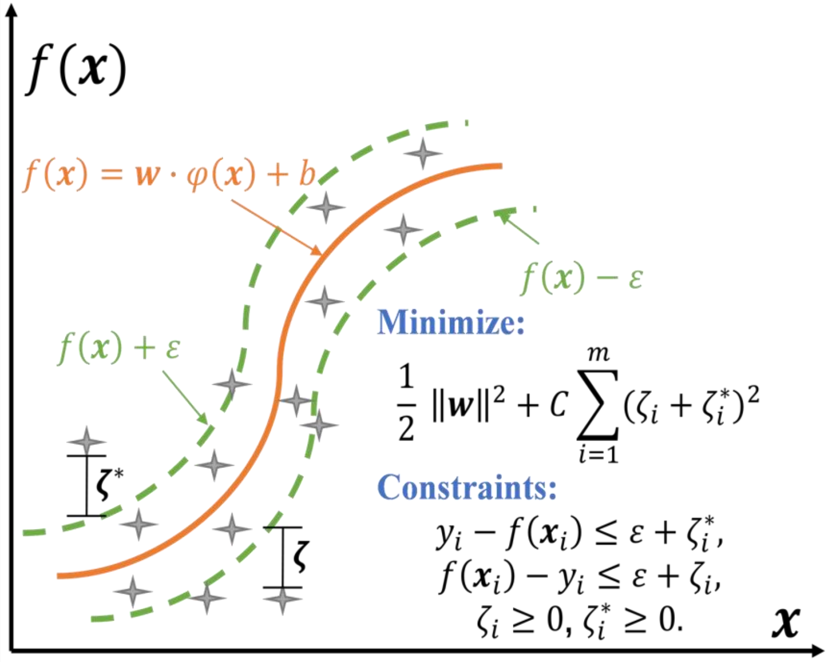
1. Main machine learning algorithms/techniques

Artificial neural network (ANN)



$$\begin{cases} \boldsymbol{a}^{(1)} = f_1(\boldsymbol{w}^{(1)}\boldsymbol{x} + \boldsymbol{b}^{(1)}) \\ \boldsymbol{a}^{(2)} = f_2(\boldsymbol{w}^{(2)}\boldsymbol{a}^{(1)} + \boldsymbol{b}^{(2)}) \\ \vdots \\ \boldsymbol{a}^{(l)} = f_l(\boldsymbol{w}^{(l)}\boldsymbol{a}^{(l-1)} + \boldsymbol{b}^{(l)}) \\ \boldsymbol{y} = f_{l+1}(\boldsymbol{w}^{(l+1)}\boldsymbol{a}^{(l)} + \boldsymbol{b}^{(l+1)}) \end{cases}$$

Support vector regression (SVR)



Minimize:

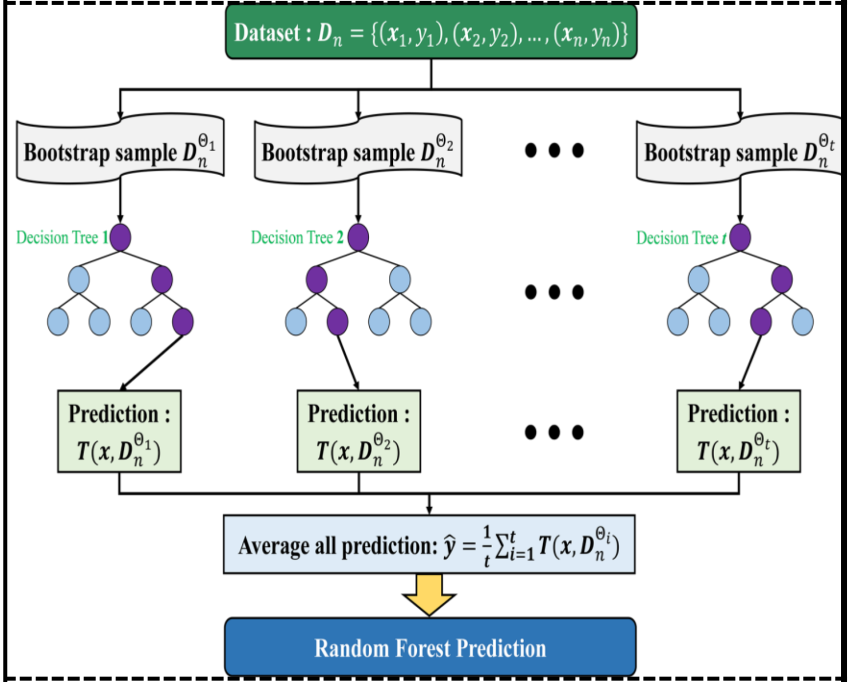
$$\frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{m}(\zeta_i + \zeta_i^*)^2$$

Constraints:

$$y_i - f(\boldsymbol{x}_i) \le \varepsilon + \zeta_i^*, \quad f(\boldsymbol{x}_i) - y_i \le \varepsilon + \zeta_i, \quad \zeta_i \ge 0, \zeta_i^* \ge 0.$$

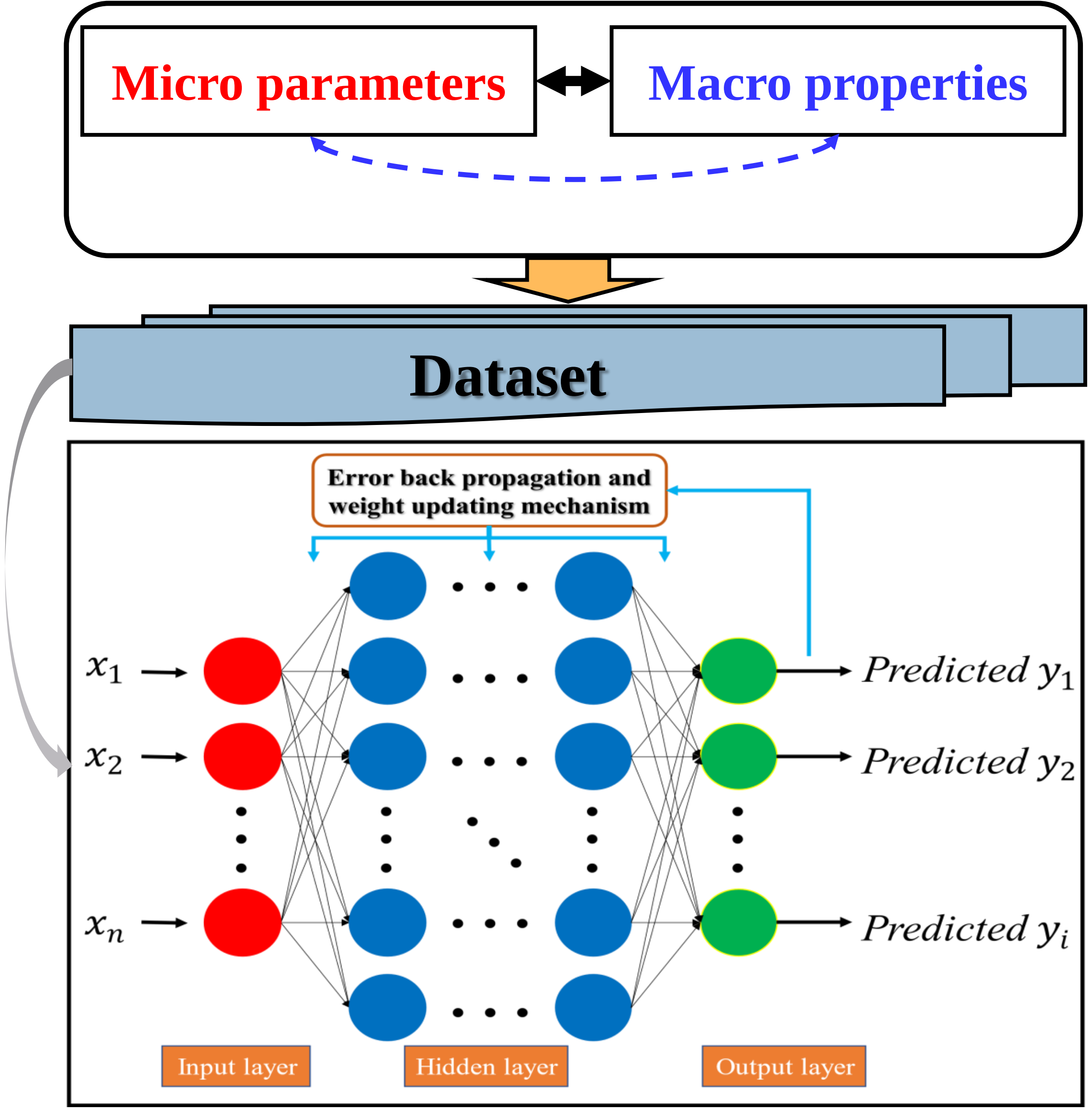
$$\begin{cases} f(\boldsymbol{x}) = \boldsymbol{w} \cdot \varphi(\boldsymbol{x}) + b \\ f(\boldsymbol{x}) = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\varphi(\boldsymbol{x}_i)\boldsymbol{x} + b \\ b = y_i + \varepsilon - \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\varphi(\boldsymbol{x}_i)\boldsymbol{x} \\ f(\boldsymbol{x}) = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*)\kappa(\boldsymbol{x}_i, \boldsymbol{x}_j) + b \end{cases}$$

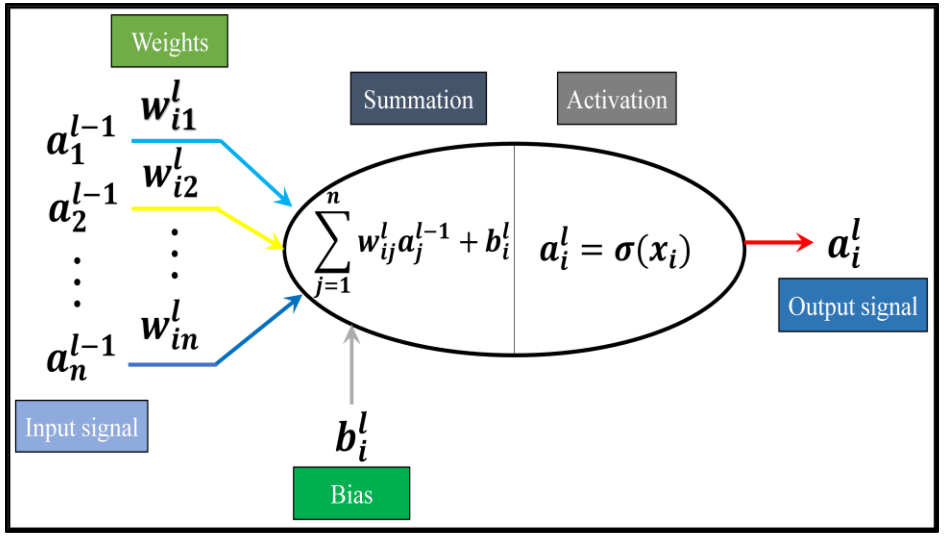
Random forest (RF)



$$\begin{cases} \boldsymbol{D}_n = \{(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), \dots, (\boldsymbol{x}_n, y_n)\} \\ \boldsymbol{D}_n^{\Theta_1}, \boldsymbol{D}_n^{\Theta_2}, \dots, \boldsymbol{D}_n^{\Theta_t} \\ T(\boldsymbol{x}, \boldsymbol{D}_n^{\Theta_1}), T(\boldsymbol{x}, \boldsymbol{D}_n^{\Theta_2}), \dots, T(\boldsymbol{x}, \boldsymbol{D}_n^{\Theta_t}) \\ \hat{y} = \frac{1}{t}\sum_{i=1}^{t} T(\boldsymbol{x}, \boldsymbol{D}_n^{\Theta_i}) \end{cases}$$

2. ANN models





ANN models:

- one input, one output, one or several hidden layers
- a specific number of neurons in each layer
- weighted summation of inputs
- producing outputs, with appropriate activation functions; $\sigma(x) = \tanh(x)$; $\sigma(x) = \max(0, x)$(ReLU), $\sigma(x) = \frac{1}{1+\exp(-x)}$ (Sigmoid), $\sigma(x) = In(1 + \exp x)$ (Softplus), $\sigma(x) = \sigma$ (linear) etc.

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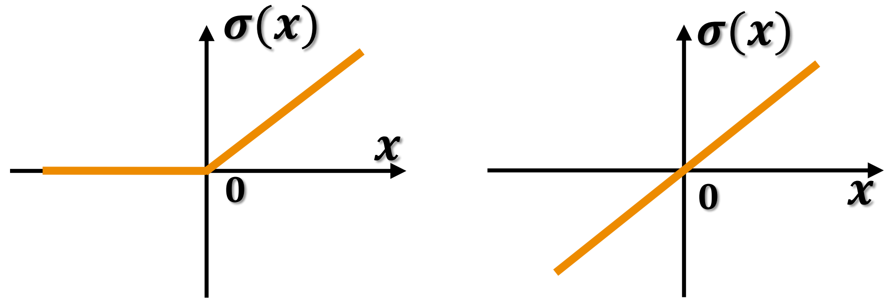
2. ANN models

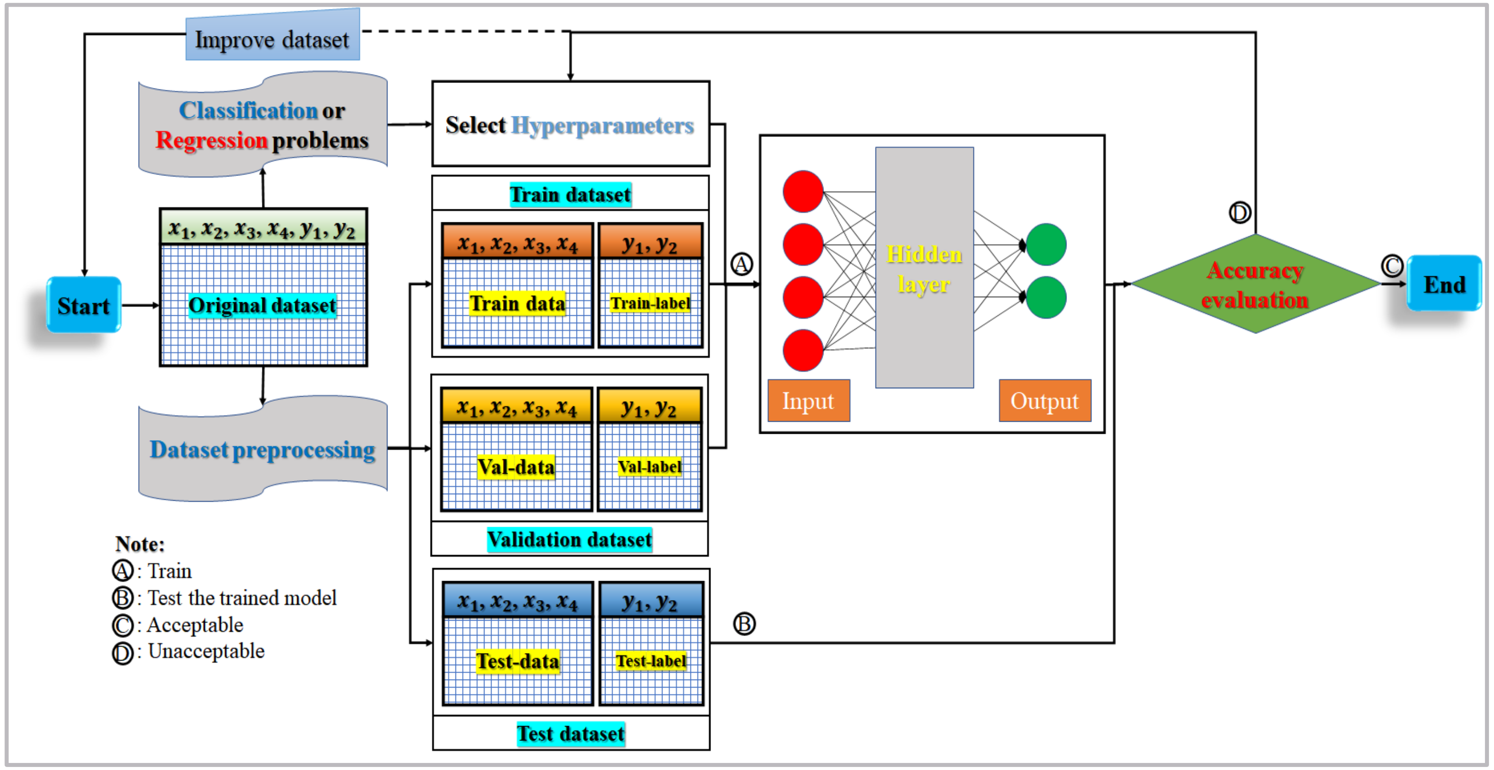
Hyperparameters:

- ✓ Number of neurons
- ✓ Number of hidden layers
- ✓ **Activation functions**
- ✓ Optimizer
- ✓ loss function
- ✓ ……

ReLU: $\sigma(x) = \max(0, x)$ linear: $\sigma(x) = x$



Activation functions

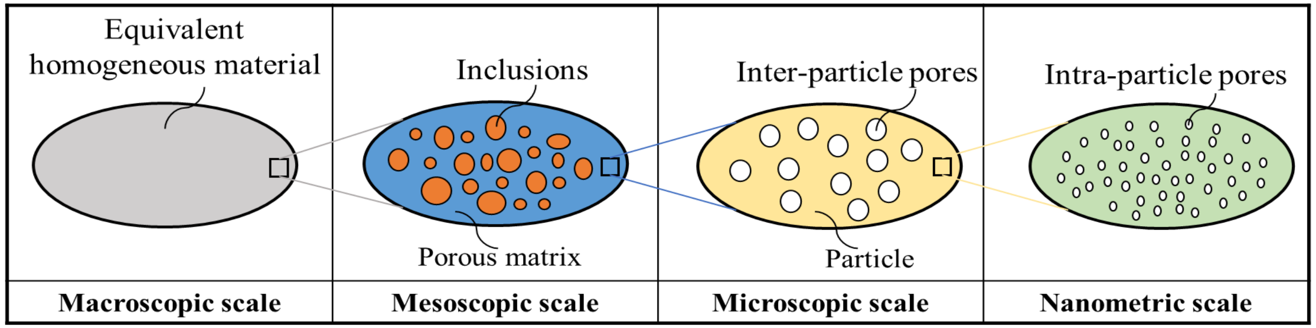


Note:
Ⓐ: Train
Ⓑ: Test the trained model
Ⓒ: Acceptable
Ⓓ: Unacceptable

Flowchart for building an ANN model

- ✓ **Learn and build nonlinear and complex relationships**
- ✓ **Infer unknown relationships between unknown data**

3.1 Analytical strength criterion and problem statement



RVE of heterogeneous materials

Drucker-Prager (DP) criterion for solid phase:

$$F^s = \tilde{\sigma}_d + T(\tilde{\sigma}_m - h) \leq 0$$

- T, **frictional coefficient** of the solid phase at the nanometric scale
- h, **hydrostatic tensile strength** of the solid phase at the nanometric scale.

Macroscopic strength criterion:

$$F = \frac{A + \frac{2B\rho}{3}}{1 + \frac{3\rho}{2} - \frac{5\rho}{6\left(\frac{A}{B}+1\right)}}\Sigma_d^2 + B\Sigma_m^2 + C\Sigma_m - \left(D + \frac{4BD + C^2}{6A}\rho\right) = 0$$

Uniaxial compression or tension:

$$\boldsymbol{\Sigma_d = R,\ \Sigma_m = (-1/3)R}$$

$$\left(\frac{A + \frac{2B\rho}{3}}{1 + \frac{3\rho}{2} - \frac{5\rho}{6\left(\frac{A}{B}+1\right)}} + \frac{B}{9}\right)R^2 - \frac{C}{3}R - \left(D + \frac{4BD + C^2}{6A}\rho\right) = 0$$

$$A = \frac{1+\frac{2f}{3}}{T^2}\left(\frac{6T^2-13f-6}{4T^2-12f-9}\phi + 1\right), B = \frac{\frac{3}{2}+f}{T^2}\phi + \frac{3f}{2T^2} - 1,$$

$$C = 2(1-f)(1-\phi)h,\ D = (1-f)^2(1-\phi)^2h^2.$$

ρ volume fraction of inclusions, ϕ large porosity, f small porosity

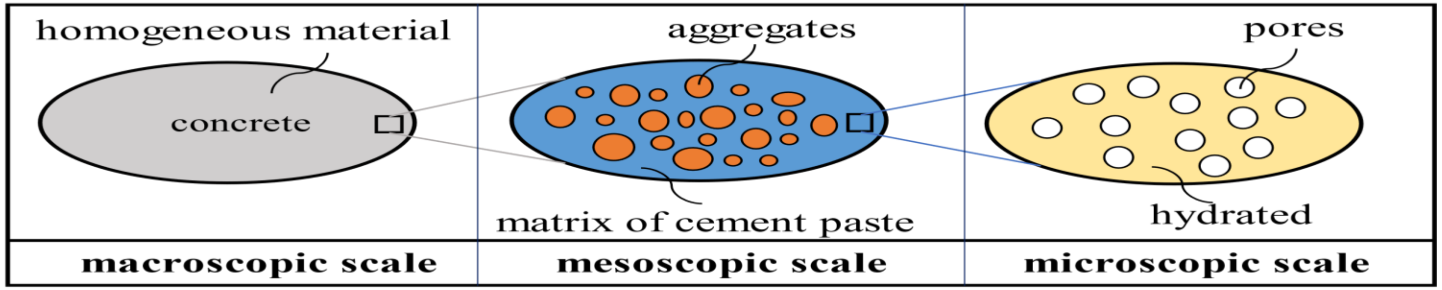
$$F(T, h, \rho, \phi, f) \longleftrightarrow R_c, R_t$$

3.2 Sensitivity analysis and simplified analytical strength criterion

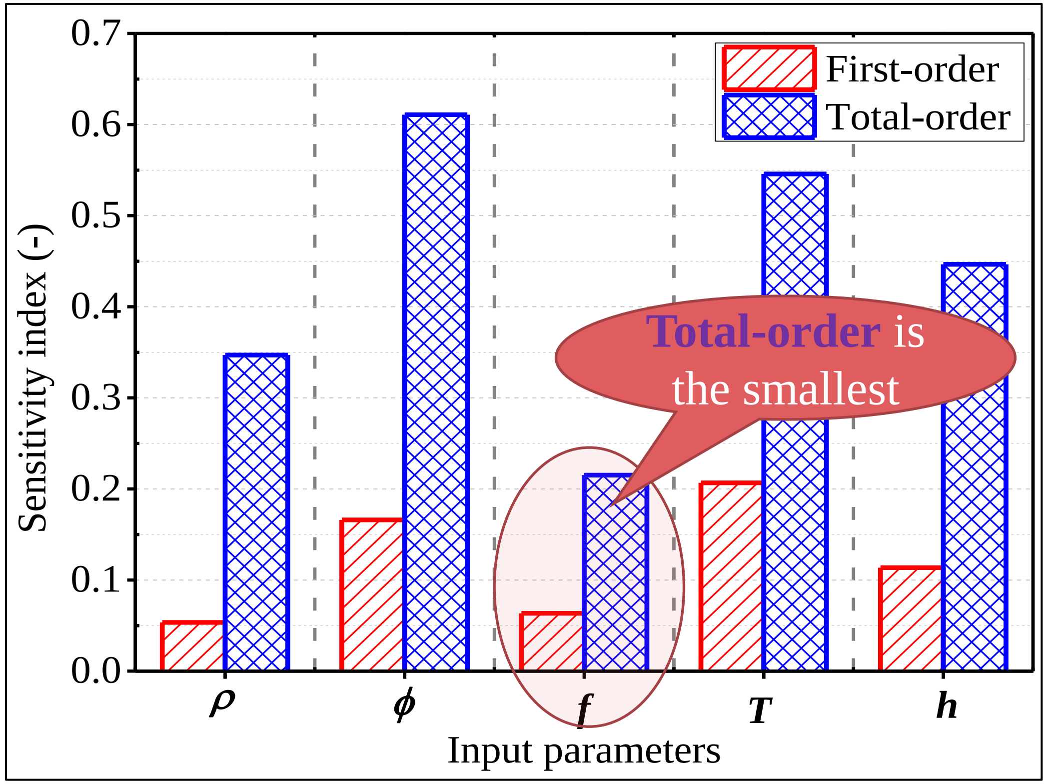
The Sobol sensitivity index:

$$S_i = \frac{V_{Xi}(E_{\boldsymbol{X}\sim i}(Y|X_i))}{V(Y)}$$

$$S_{Ti} = 1 - \frac{V_{\boldsymbol{X}\sim i}(E_{Xi}(Y|\boldsymbol{X}_{\sim i}))}{V(Y)} = \frac{E_{\boldsymbol{X}\sim i}(V_{Xi}(Y|\boldsymbol{X}_{\sim i}))}{V(Y)}$$



Simplified RVE of material



First-order and total-order index

$$\left(\frac{A' + \frac{2B'\rho}{3}}{1 + \frac{3\rho}{2} - \frac{5\rho}{6\left(\frac{A'}{B'} + 1\right)}} + \frac{B'}{9}\right) R^2 - \frac{C'}{3} R - \left(D' + \frac{4B'D' + C'^2}{6A'}\rho\right) = 0$$

$$A' = \frac{1}{T'^2}\left(\frac{6T'^2 - 6}{4T'^2 - 9}\phi + 1\right),\ B' = \frac{3}{2T'^2}\phi - 1,$$

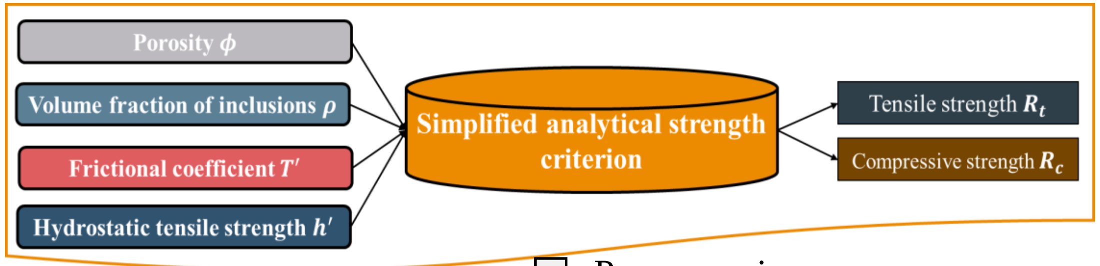
$$C' = 2(1-\phi)h',\ D' = (1-\phi)^2 h'^2.$$

***T'*, frictional coefficient of the solid phase at the microscopic** scale

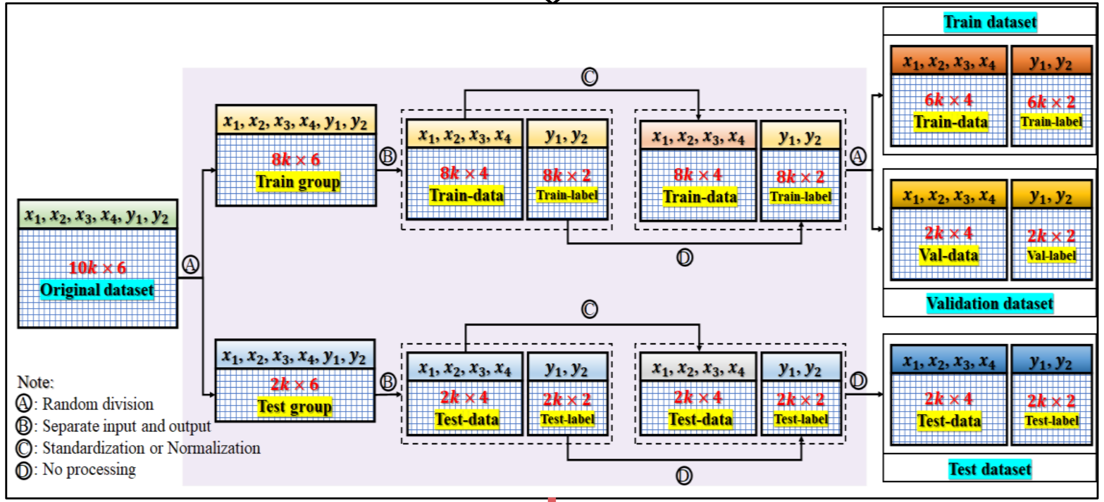
***h'* , hydrostatic tensile strength** of the solid phase at the microscopic scale

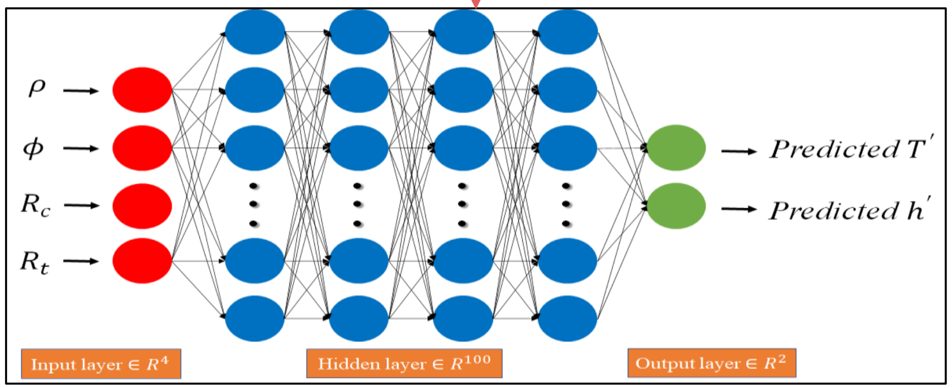
$$T', h', \rho, \phi \quad \Leftrightarrow \quad R_c, R_t$$

3.3 An ANN model for predicting T′ and h′



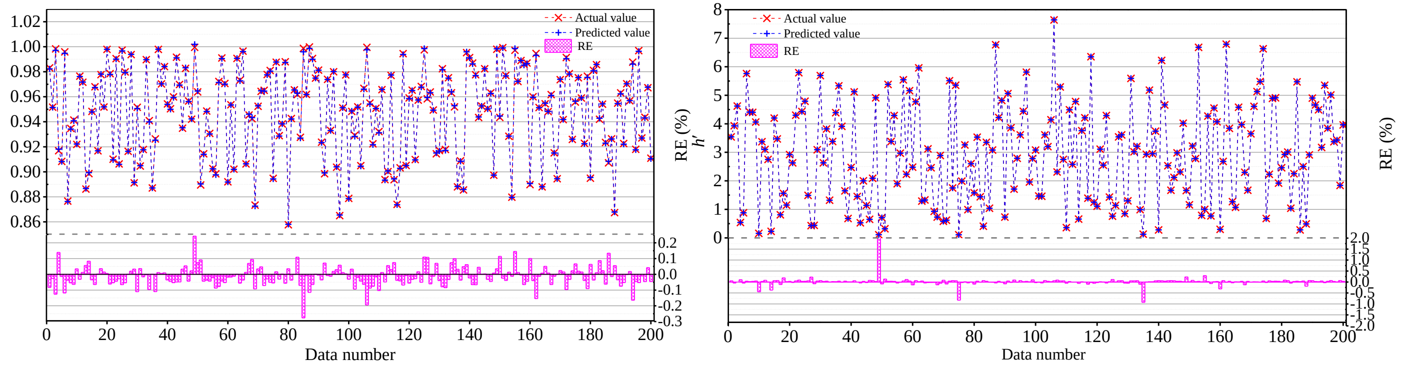
Preprocessing

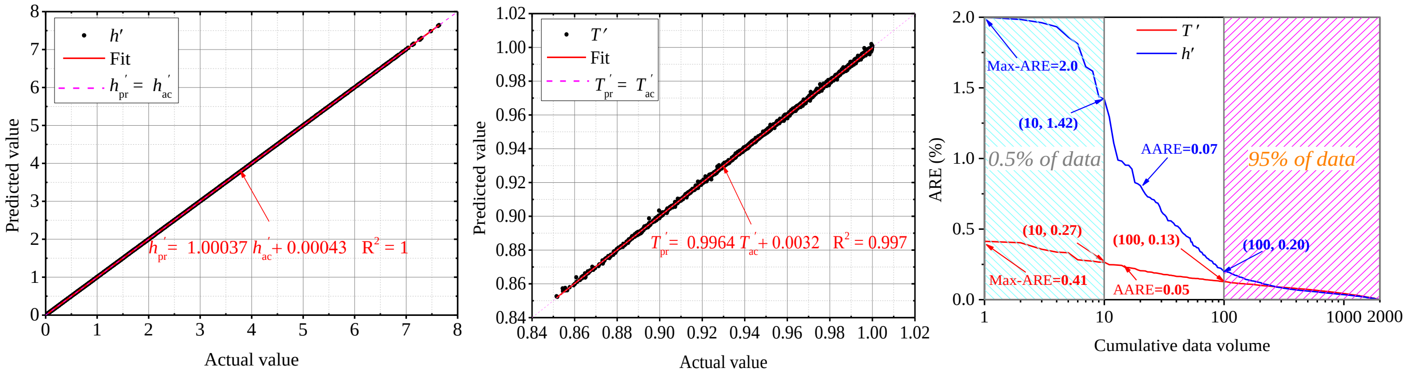




Hyper-parameters of the ANN for prediction of T' and h'

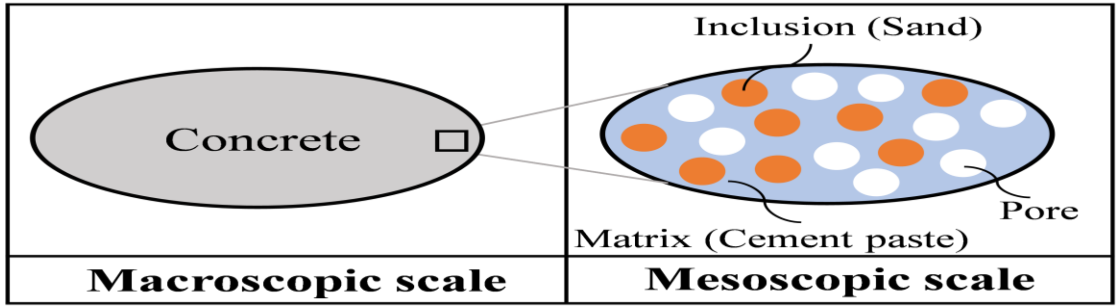
Input layer	Hidden layer	Output layer	Loss function	Optimizer
ρ, ϕ, R_c, R_t	$4 \times 100 \times$ ReLU	T', h'	MSE	Adam





- **Maximum absolute relative error** (Max-ARE)
- **Average absolute relative error** (AARE)
- **Absolute relative error** (ARE)
- **Correlation coefficient** (R^2)

4.1 Analytical bounds and estimates of elastic properties



- **Voigt bounds:**

$$\kappa_{hom} = \sum_{r=0}^{N} f_r \kappa_r \quad \mu_{hom} = \sum_{r=0}^{N} f_r \mu_r$$

- **Reuss bounds:**

$$\kappa_{hom} = (\sum_{r=0}^{N} \frac{f_r}{\kappa_r})^{-1} \quad \mu_{hom} = (\sum_{r=0}^{N} \frac{f_r}{\mu_r})^{-1}$$

- **Hashin-Shtrikman bounds:**

$$\kappa_{hom} = (\sum_{r=0}^{N} \frac{f_r \kappa_r}{3\kappa_r + 4\mu_j})(\sum_{r=0}^{N} \frac{f_r}{3\kappa_r + 4\mu_j})^{-1}$$

$$\mu_{hom} = (\sum_{r=0}^{N} \frac{f_r \mu_r}{\mu_j(9\kappa_j + 8\mu_j) + 6\mu_r(\kappa_j + 2\mu_j)})(\sum_{r=0}^{N} \frac{f_r}{\mu_j(9\kappa_j + 8\mu_j) + 6\mu_r(\kappa_j + 2\mu_j)})^{-1}$$

- **Mori-Tanaka scheme:**

$$\kappa_{hom} = (f_0 \kappa_0 + \sum_{r=1}^{N} \frac{f_r \kappa_r \kappa_0}{\kappa_0 + 3\gamma_0(\kappa_r - \kappa_0)})(f_0 + \sum_{r=1}^{N} \frac{f_r \kappa_0}{\kappa_0 + 3\gamma_0(\kappa_r - \kappa_0)})^{-1}$$

$$\mu_{hom} = (f_0 \mu_0 + \sum_{r=1}^{N} \frac{f_r \mu_r \mu_0}{\mu_0 + 2\delta_0(\mu_r - \mu_0)})(f_0 + \sum_{r=1}^{N} \frac{f_r \mu_0}{\mu_0 + 2\delta_0(\mu_r - \mu_0)})^{-1}$$

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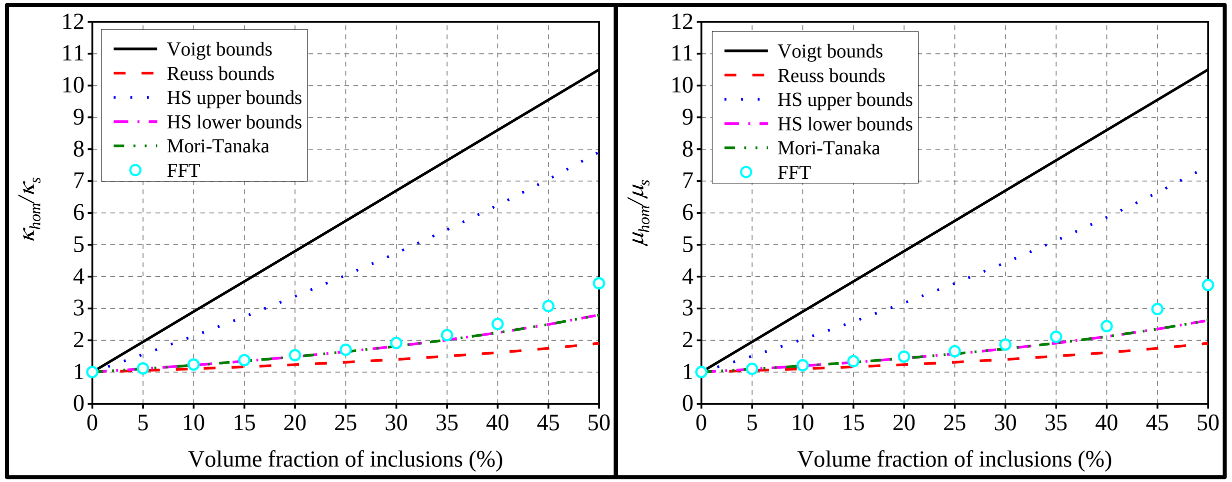
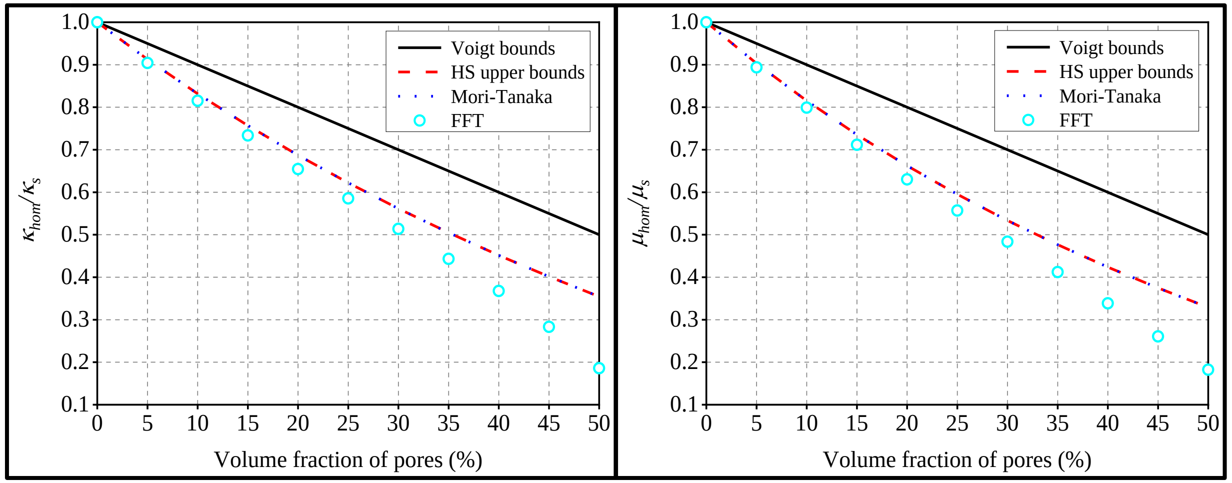
4.1 Analytical bounds and estimates of elastic properties

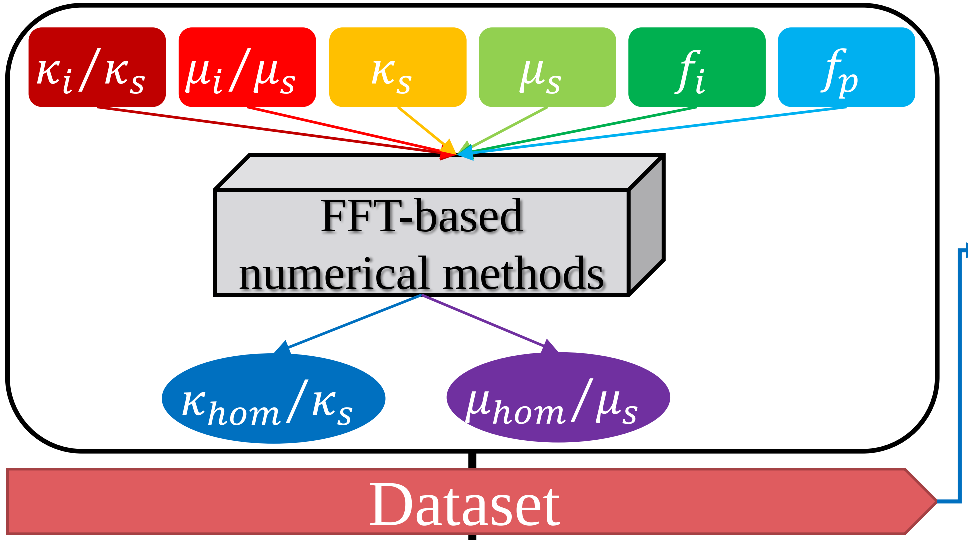


(Only inclusions)



Only pores

4.2 An ANN based model

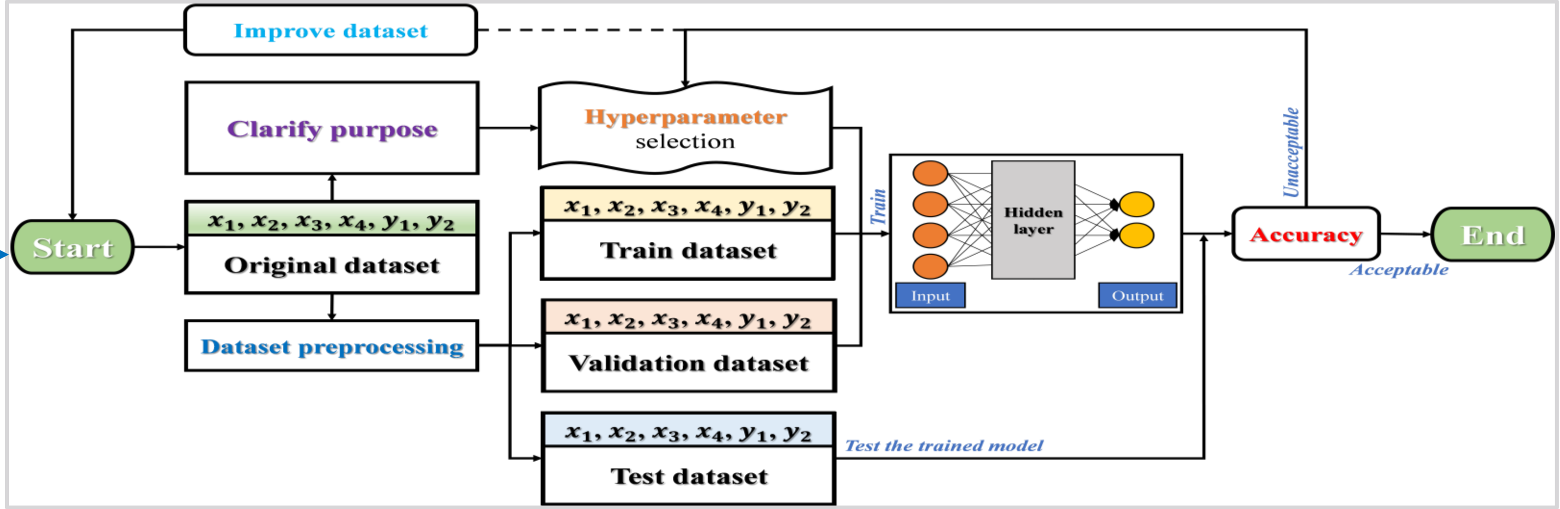


κ_i/κ_s μ_i/μ_s κ_s μ_s f_i f_p

FFT-based numerical methods

κ_{hom}/κ_s μ_{hom}/μ_s

Dataset



Improve dataset

Start

Clarify purpose

$x_1, x_2, x_3, x_4, y_1, y_2$

Original dataset

Dataset preprocessing

Hyperparameter selection

$x_1, x_2, x_3, x_4, y_1, y_2$

Train dataset

$x_1, x_2, x_3, x_4, y_1, y_2$

Validation dataset

$x_1, x_2, x_3, x_4, y_1, y_2$

Test dataset

Train

Hidden layer

Input

Output

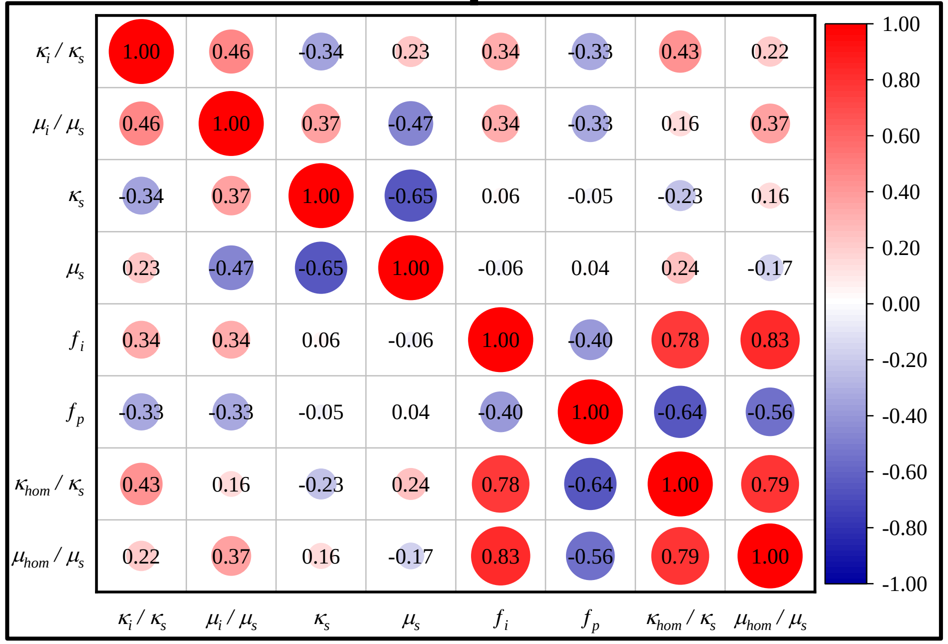
Test the trained model

Unacceptable

Accuracy

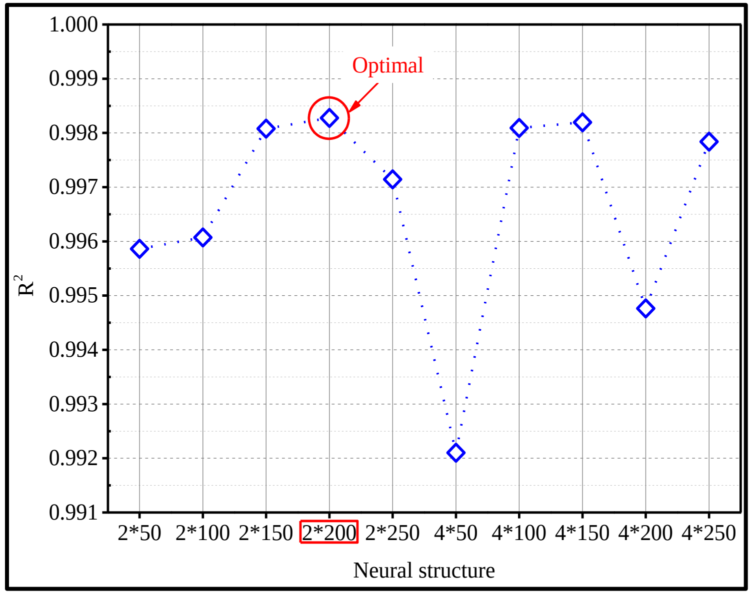
Acceptable

End

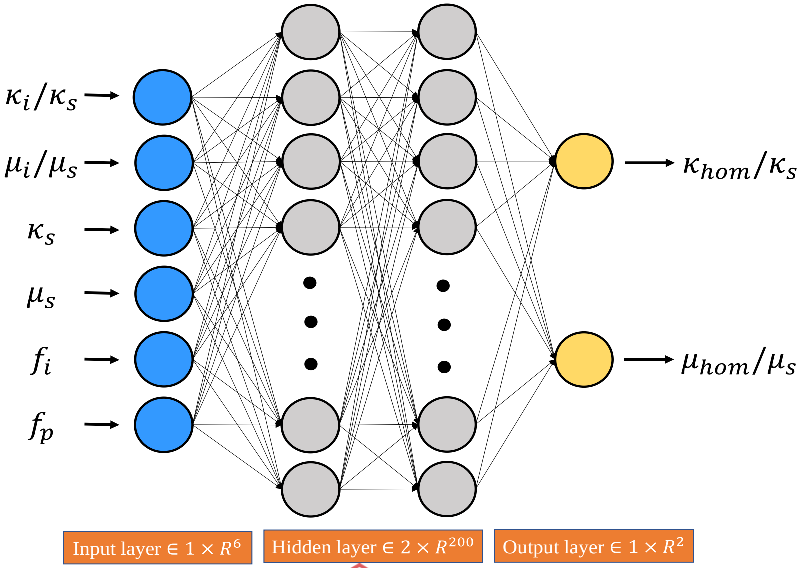


	κ_i/κ_s	μ_i/μ_s	κ_s	μ_s	f_i	f_p	κ_{hom}/κ_s	μ_{hom}/μ_s
κ_i/κ_s	1.00	0.46	-0.34	0.23	0.34	-0.33	0.43	0.22
μ_i/μ_s	0.46	1.00	0.37	-0.47	0.34	-0.33	0.16	0.37
κ_s	-0.34	0.37	1.00	-0.65	0.06	-0.05	-0.23	0.16
μ_s	0.23	-0.47	-0.65	1.00	-0.06	0.04	0.24	-0.17
f_i	0.34	0.34	0.06	-0.06	1.00	-0.40	0.78	0.83
f_p	-0.33	-0.33	-0.05	0.04	-0.40	1.00	-0.64	-0.56
κ_{hom}/κ_s	0.43	0.16	-0.23	0.24	0.78	-0.64	1.00	0.79
μ_{hom}/μ_s	0.22	0.37	0.16	-0.17	0.83	-0.56	0.79	1.00

Pearson correlation coefficient



Model structure choice



Input layer $\in 1 \times R^6$

Hidden layer $\in 2 \times R^{200}$

Output layer $\in 1 \times R^2$

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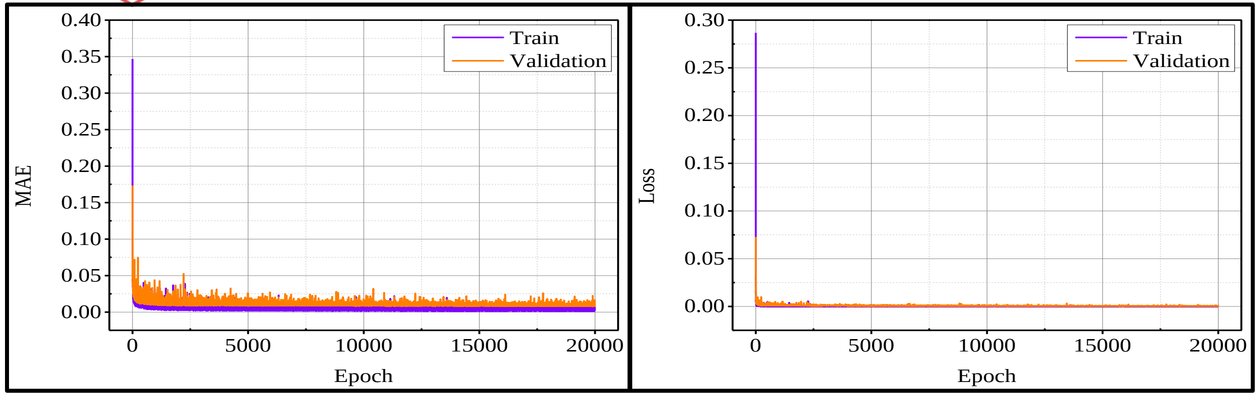
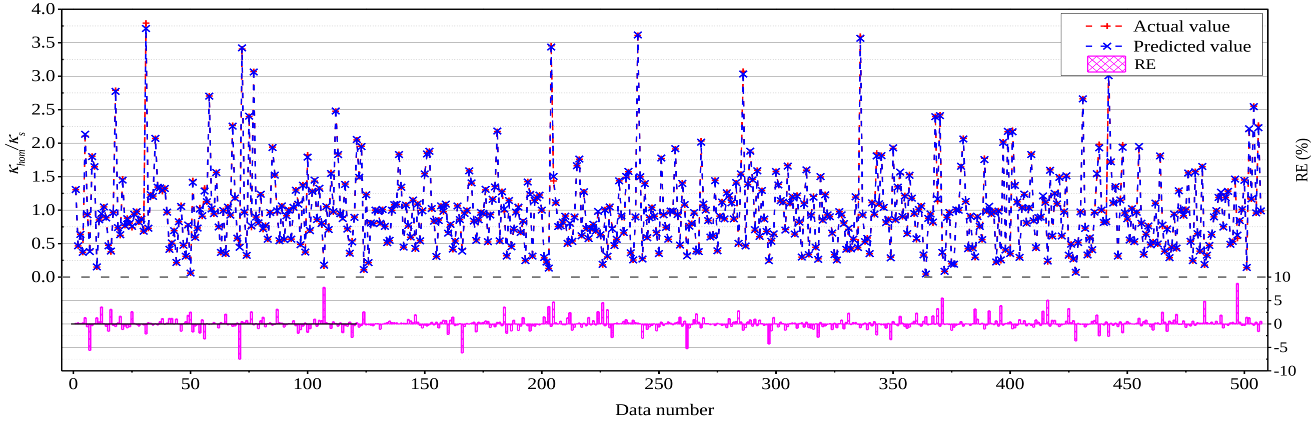
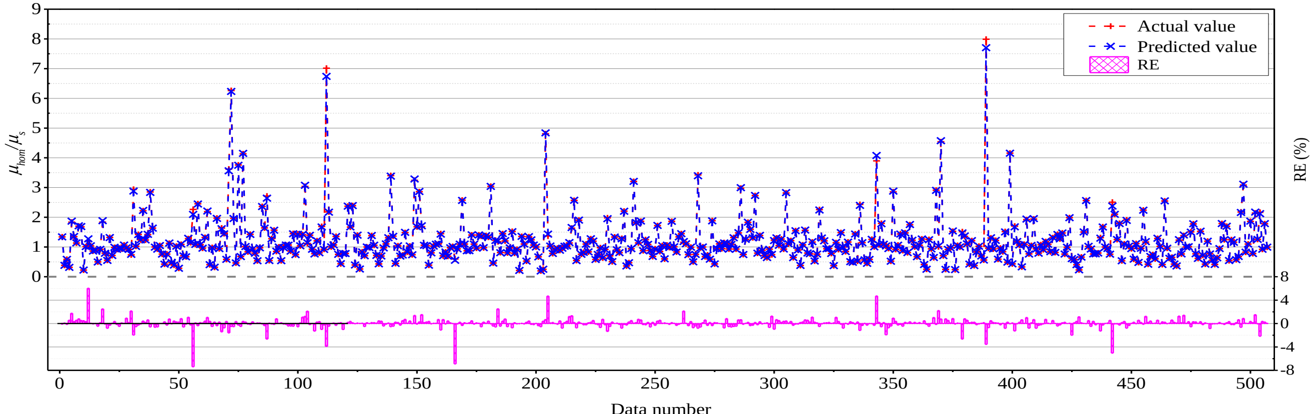
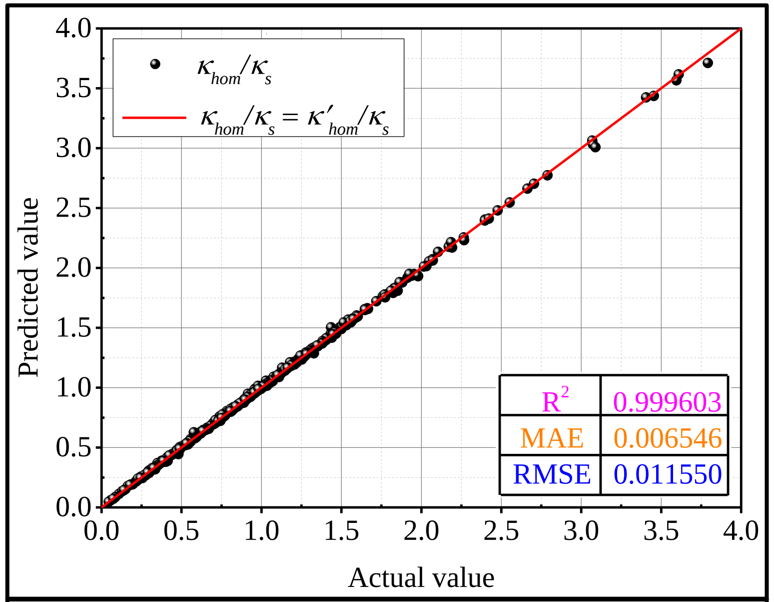
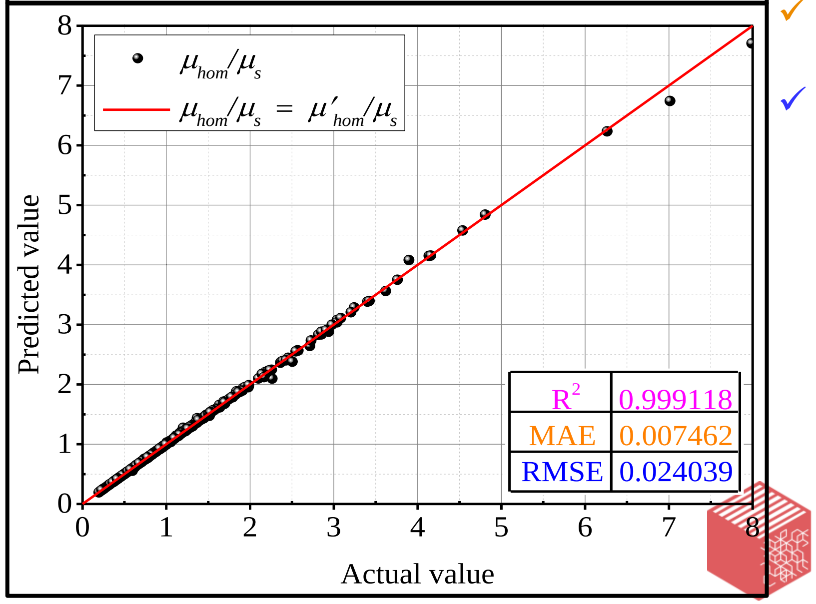
4.3 ANN model assessment











Metrics

- ✓ **RE: Relative error**
- ✓ **R^2: Coefficient of determination**
- ✓ **MAE: Mean absolute error**
- ✓ **RMSE: Root mean squared error**

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5. Conclusions and ongoing work

1. Conclusions

- ✓ **ANN based models** are able to accurately not only identify microscopic properties, but also estimate macroscopic properties of complex heterogeneous materials;
- ✓ **Combination of ML based and micromechanical models** provides a powerful tool to understand relationships between micro-structures and macroscopic properties.

2. Ongoing studies

- ☐ Enrichment of dataset from direct simulations of complex micro-structures and laboratory tests with controlled micro-structures, estimation of **macroscopic strength properties and their uncertainty;**
- ☐ **Determination of stress-strain relations directly by ML based models;**
- ☐ Combination with 3D printing technology, smart materials design for specific requirements.

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