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Prediction of thermal conductivity of polymer-based composites by using SVR

Linear Algebra and polymer applications

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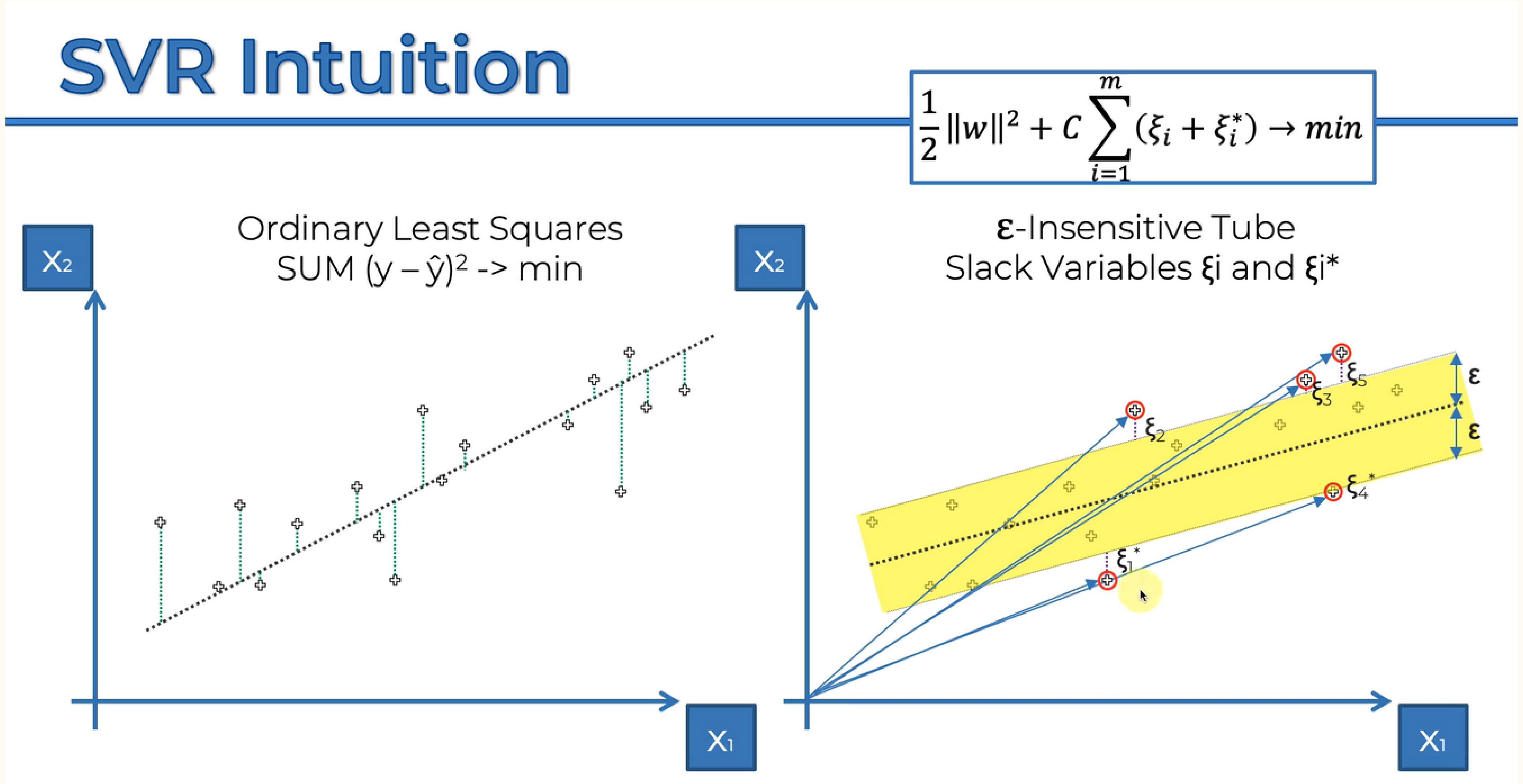
WHY?

- **Thermal conductivity** is vital for many applications polymer-based composites (aerospace, automobile industry, textile and chemical industry, etc) because most polymers have low thermal conductivity. Introducing conductive fillers can enhance their performance, making them useful in aerospace, automobile, textile, and chemical industries, among others.
- So far two theoretical models (flake and spherical packing) have been developed to simulate the thermal conductivity of three-phase polymer composites with varying mass fractions of copolymer Styrene-ethylene-butylene-styrene(SEBS), polyethylene (PE), and polystyrene (PS) but due to mean absolute percentage errors (MAPE) calculated by the two models were over ~8% their is need to device a more accurate model.

HOW?

- Using support vector regression (SVR) with particle swarm optimization (PSO) and leave-one-out cross-validation (LOOCV) to model and predict the thermal conductivity of three-phase polymer composites

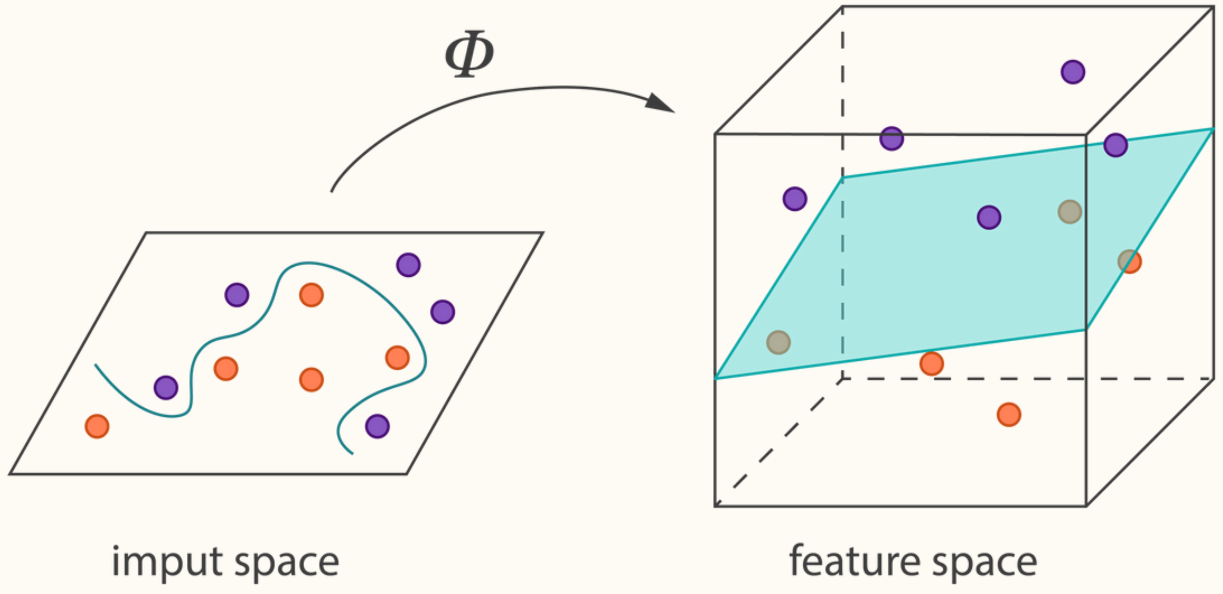
SVR in picture!



m = is the number of training samples
C = penalty factor
epsilon = prescribed parameter controlling the tolerance to error

- (1/2)||w||2 is used as a flatness measurement of function.

  second is insensitive loss function



kernels

"A kernel function is a mathematical function that transforms the input data into a higher dimensional feature space."

MATHS BEHIND

nonlinear mapping Φ(x)

$$f(\boldsymbol{x}) = \boldsymbol{w} \cdot \Phi(\boldsymbol{x}) + b, \quad \Phi : \boldsymbol{R}^N \to \boldsymbol{F}, \boldsymbol{w} \in \boldsymbol{F}, \tag{1}$$

$$\text{minimize } R(C) = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{m} L_\varepsilon(f(\boldsymbol{x}_i) - y_i), \tag{2}$$

$$L_\varepsilon(f(\boldsymbol{x}_i) - y_i) = \begin{cases} 0, \text{ if } |f(\boldsymbol{x}_i) - y_i| \leqslant \varepsilon, \\ |f(\boldsymbol{x}_i) - y_i| - \varepsilon, \text{ if } |f(\boldsymbol{x}_i) - y_i| > \varepsilon. \end{cases} \tag{3}$$

regularized risk function:

$$R(\boldsymbol{w}, \xi_i, \xi_i^*) = \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{m}(\xi_i + \xi_i^*),$$
$$\text{subject to } \begin{cases} y_i - \boldsymbol{w} \cdot \boldsymbol{x}_i - b \leqslant \varepsilon + \xi_i, \\ \boldsymbol{w} \cdot \boldsymbol{x}_i + b - y_i \leqslant \varepsilon + \xi_i^*, \\ \xi_i, \xi_i^* \geqslant 0. \end{cases} \tag{4}$$

primal function

$$\begin{aligned} L(\boldsymbol{w}, \xi_i, \xi_i^*) = {} & \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_{i=1}^{m}(\xi_i + \xi_i^*) \\ & - \sum_{i=1}^{m}\alpha_i((\varepsilon + \xi_i) + y_i + (\boldsymbol{w} \cdot \Phi(\boldsymbol{x}_i)) + b) \\ & - \sum_{i=1}^{m}\alpha_i^*((\varepsilon + \xi_i^*) + y_i + (\boldsymbol{w} \cdot \Phi(\boldsymbol{x}_i)) - b) \\ & - \sum_{i=1}^{m}(\lambda_i\xi_i + \lambda_i^*\xi_i^*), \end{aligned} \tag{5}$$

Lagrange equation

$$\frac{\partial L}{\partial \boldsymbol{w}} = \boldsymbol{w} - \sum_{i=1}^{m}(\alpha_i - \alpha_i^*) \cdot \Phi(\boldsymbol{x}_i) = 0,$$
$$\frac{\partial L}{\partial b} = \sum_{i=1}^{m}(\alpha_i - \alpha_i^*) = 0,$$
$$\frac{\partial L}{\partial \xi_i} = C - \alpha_i - \lambda_i = 0,$$
$$\frac{\partial L}{\partial \xi_i^*} = C - \alpha_i^* - \lambda_i^* = 0.$$

Radial Kernal function

$$\boldsymbol{w} = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)\Phi(\boldsymbol{x}_i), \tag{8}$$

$k(\boldsymbol{x}, \boldsymbol{x}_i) = \Phi(\boldsymbol{x}) \cdot \Phi(\boldsymbol{x}_i)$ is a kernel function.

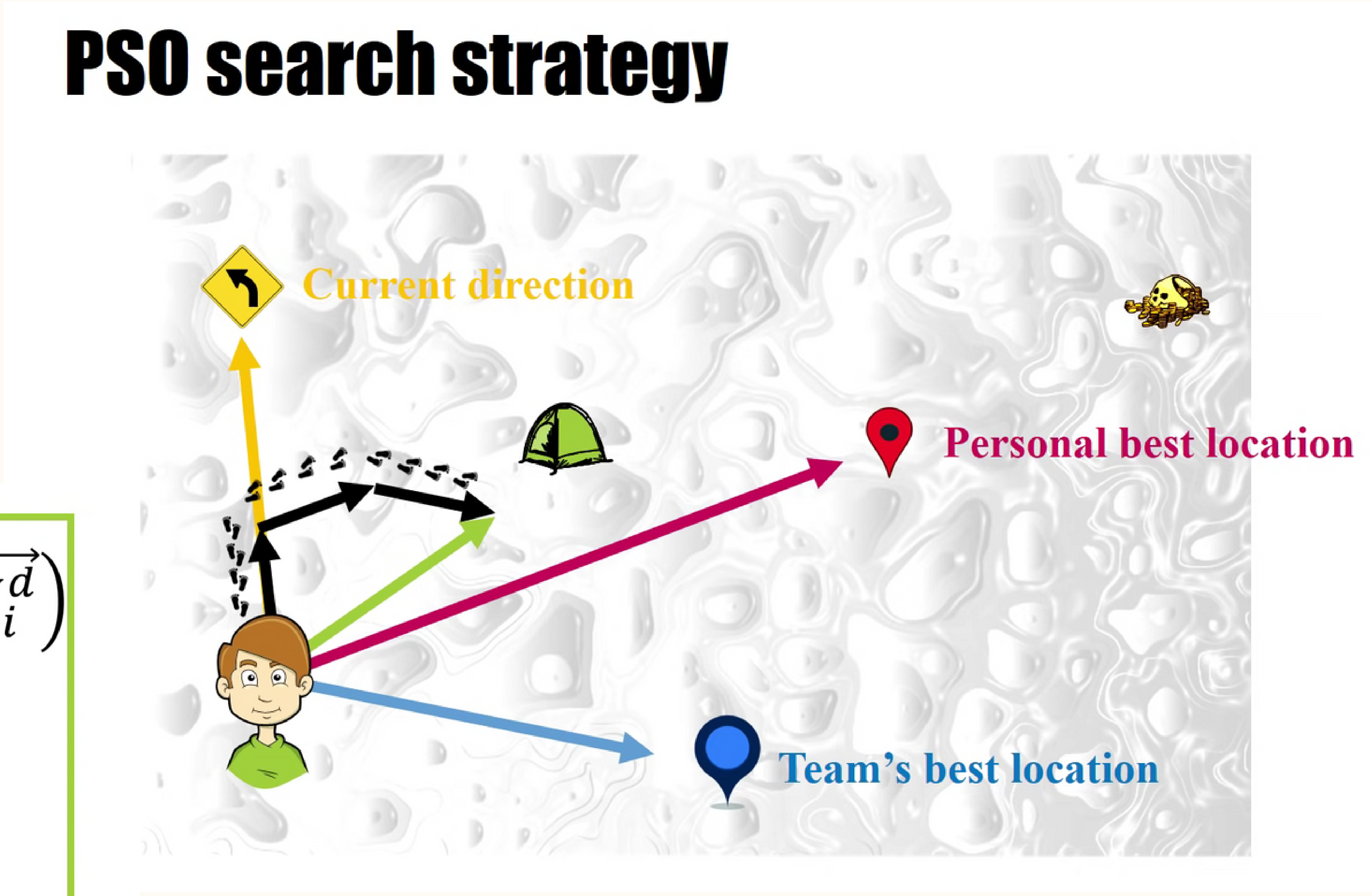
$$k(\boldsymbol{x}, \boldsymbol{x}_i) = \exp(-\gamma\|\boldsymbol{x} - \boldsymbol{x}_i\|^2). \tag{10}$$

Final linear equation

$$f(\boldsymbol{x}) = \sum_{i=1}^{l}(\alpha_i - \alpha_i^*)k(\boldsymbol{x}, \boldsymbol{x}_i) + b, \tag{9}$$

PSO (particle swarm optimization)

Searching treasure analogy



$$\overrightarrow{V_i^{d+1}} = 2r_1 \overrightarrow{V_i^{d}} + 2r_2\left(\overrightarrow{P_i^{d}} - \overrightarrow{X_i^{d}}\right) + 2r_3\left(\overrightarrow{G^{d}} - \overrightarrow{X_i^{d}}\right)$$

Next velocity (tomorrow)

Current velocity (today)

Personal best solution

Global best solution

Distance to the personal best

Distance to the global best

PSO

- Optimization of SVR parameters (ε, C, γ) is crucial for its generalization ability
- Particle Swarm Optimization (PSO) algorithm is used to find the optimal parameter subset
- PSO adjusts the velocity and location of particles in the 3D space of parameter vectors (ε, C, γ)
- Each particle represents a subset and has a local best-fit value (Pibest) and global best-fit value (Gbest)
- The iterative equations for adjusting the velocity and position of particles are shown

$$\boldsymbol{v}_i(t+1) = \omega \boldsymbol{v}_i(t) + c_1 \mathrm{rand}()(\boldsymbol{p}_{i\mathrm{best}} - \boldsymbol{u}_i(t)) + c_2 \mathrm{rand}()(\boldsymbol{g}_{\mathrm{best}} - \boldsymbol{u}_i(t)),$$

$$\boldsymbol{u}_i(t+1) = \boldsymbol{u}_i(t) + \boldsymbol{v}_i(t+1),$$

- Learning factors c1 and c2 are set as 2, and the weighting factor ω is automatically regulated with the iterative time of the algorithm
- Mean Absolute Percentage Error (MAPE) is used as the fitness function to reflect the performance of SVR

$$\mathrm{MAPE} = \frac{1}{m} \sum_{i=1}^{m} \left| \frac{\hat{y}_i - y_i}{y_i} \right|.$$

Modeling strategy

- Support Vector Regression (SVR) via leave-one-out cross-validation (LOOCV) was applied to model and predict the thermal conductivity by using the dataset.
- Weight percent of SEBS, PS and PE are considered, one of the three input factors should be excluded during the modelling process so as to attain a reasonable and accurate SVR model.
- Input factors for SVR modeling - mass fractions of PE and PS
- Output variable for SVR modeling - thermal conductivity of composite.

Evaluation of model’s generalization performance

- Mean absolute percentage error (MAPE), mean absolute error (MAE) and correlation coefficients (R^2) are used to evaluate the performance of regression models.

Formula used

$$MAE = \frac{1}{n}\sum_{j=1}^{n}\left|\hat{y}_j - y_j\right|,$$

$$R^2 = \frac{\left(\sum_{j=1}^{n}(\hat{y}_j - \bar{\hat{y}})(y_j - \bar{y})\right)^2}{\left(\sum_{j=1}^{n}(\hat{y}_j - \bar{\hat{y}})^2 \cdot \sum_{j=1}^{n}(y_j - \bar{y})^2\right)},$$

where, n represents the total number of test samples, yj stands for the experimental value (or target value) and ˆyj denotes the predicted value for the jth test sample, and mean target value as well as the mean predicted value for all test samples.

Results and Conclusion

- Compared the values of k, MAE, MAPE, and R^2 of the prediction performance for the flake packing model, Spherical packing mode, and LOOCV test of SVR.

Method	MAE ($W\ m^{-1}\ K^{-1}$)	MAPE (%)	R^2
Flake packing model [23]	0.0168	8.72	0.9253
Spherical packing model [23]	0.0165	8.60	0.9241
SVR-LOOCV	0.0034	0.96	0.9954

- The addition of polymer PE with higher thermal conductivity can efficiently increase the thermal conductivity of the polymer matrix composite.
- For one test sample, the error of SVR for this sample is slightly greater than that of either the flake packing model or spherical packing model. This case revealed that the SVR has a limited extrapolation capacity than those of the theoretical models.

Conclusion:

MAE and MAPE based on the LOOCV test of SVR models are the smallest indicating SVR has a theoretical significance. Increasing the size of the training dataset can help to improve the generalization ability of the SVR model

Refrences

Wang, GuiLian, et al. "Prediction of thermal conductivity of polymer-based composites by using support vector regression." Science China Physics, Mechanics and Astronomy 54 (2011): 878-883.

Thank You