Indian Institute of Technology, Bombay

Course Project (ME793)

Finding Additive Manufacturing process parameters for optimum properties

Fused deposition modelling of high-performance thermoplastic polymer - Polyether ether ketone (PEEK)

Under guidance of
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Motivation

- Additive manufacturing(AM) is most advanced type of manufacturing process, it reduces waste and save more than 50% of energy compared to today's subtractive manufacturing process and reduce material costs by up to 90%.
- The fabrication of UAVs and different aviation parts has attracted a lot of attention in the use of additive manufacturing methods. AM offers designers the freedom to create intricate structures that are difficult to create using traditional techniques [1].
- The aircraft industry has significantly expanded its use of thermoplastic composite materials in recent years. Their benefits, including recyclability, weldability, fast production, great resistance to chemical and physical deterioration, long shelf life, etc., are the driving factors [2] .
- This motivated us to study the effect of process parameter of Fused Deposition Modeling(most popular, fast and cheap method of AM for thermoplastic polymer) on carbon-fiber reinforced thermoplastic polymer composite material.

Objective

- To optimize multiple properties given a single/multiple process parameters.
- To optimize a single property by using all of the process parameter and check for the dominant parameters driving that property.

Properties and process parameters to be studied:

Tensile strength: nozzle diameter, infill angle, nozzle temperature, printing speed, plate form temperature, chamber temperature, layer thickness, raster angle.

Surface roughness: printing speed, layer thickness, nozzle temperature, infill percentage, nozzle diameter.

Elastic modulus: Nozzle temperature, printing speed, layer thickness, infill percentage, platform temperature.

Flexural strength: Chamber temperature, nozzle temperature, printing speed, plate form temperature.

Preliminary data analysis plots

Scatter plots fitted with 2-degree polynomial trend line

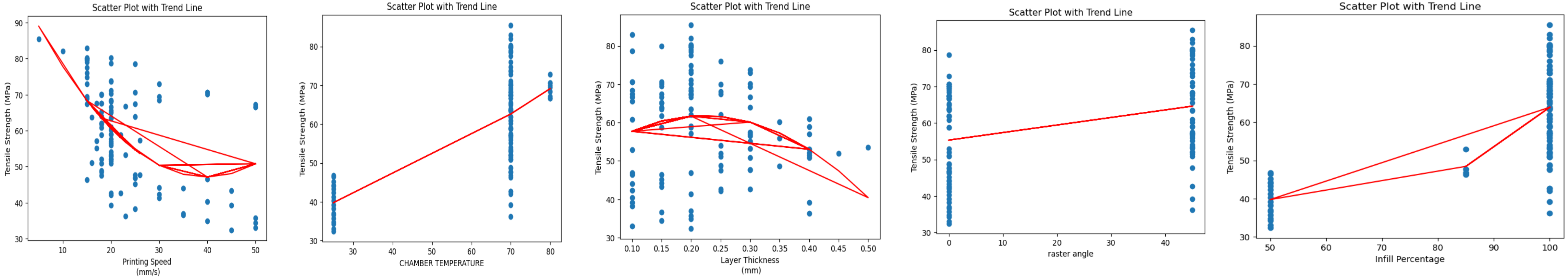

Fig 1: Scatter plot for tensile strength vs important process parameters

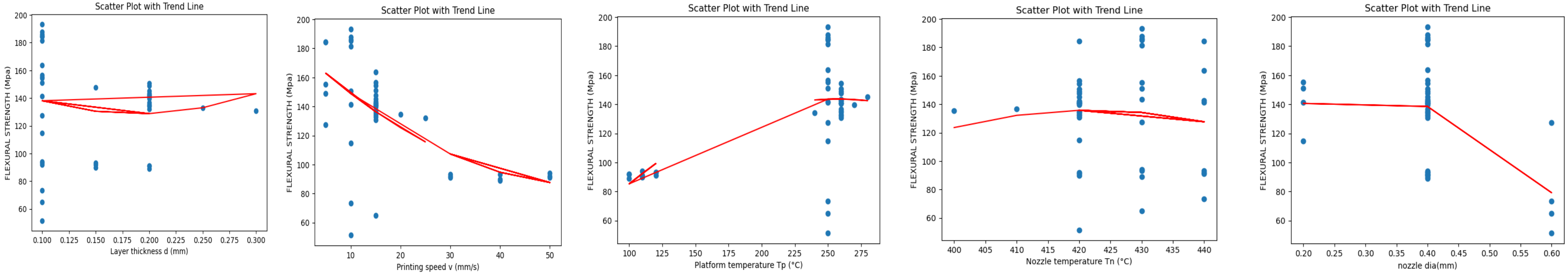

Fig 2: Scatter plot for flexural strength vs important process parameters

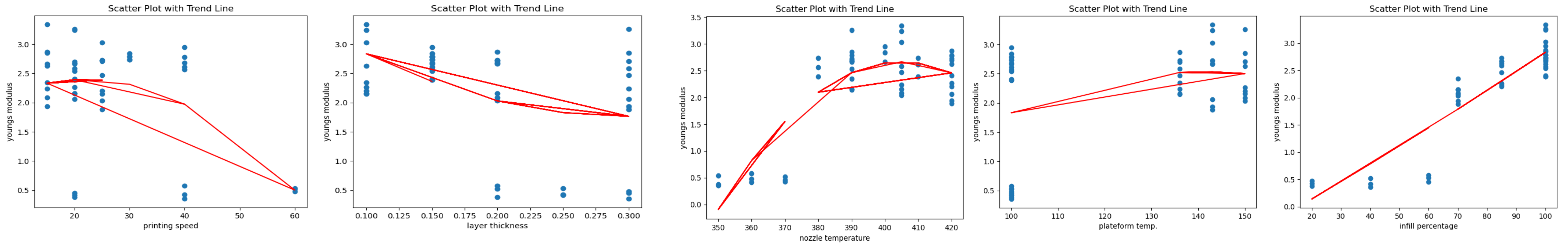

Fig 3: Scatter plot for elastic modulus under tension vs important process parameters

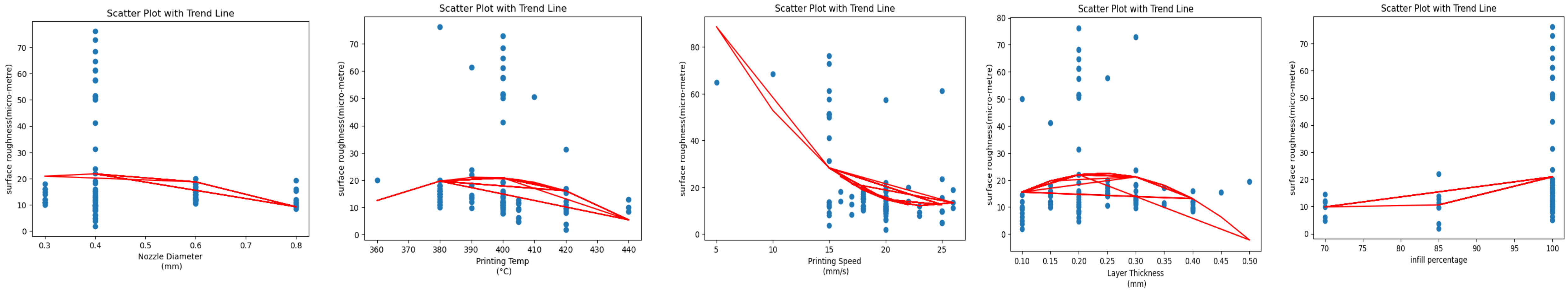

Fig 4: Scatter plot for surface roughness vs important process parameters

$$r = 1 - \frac{6\sum d^2}{n(n^2 - 1)}$$

r - is the Spearman correlation coefficient

$\sum d^2$- is the sum of the squared differences between the ranks of the paired observations

n - is the number of paired observations

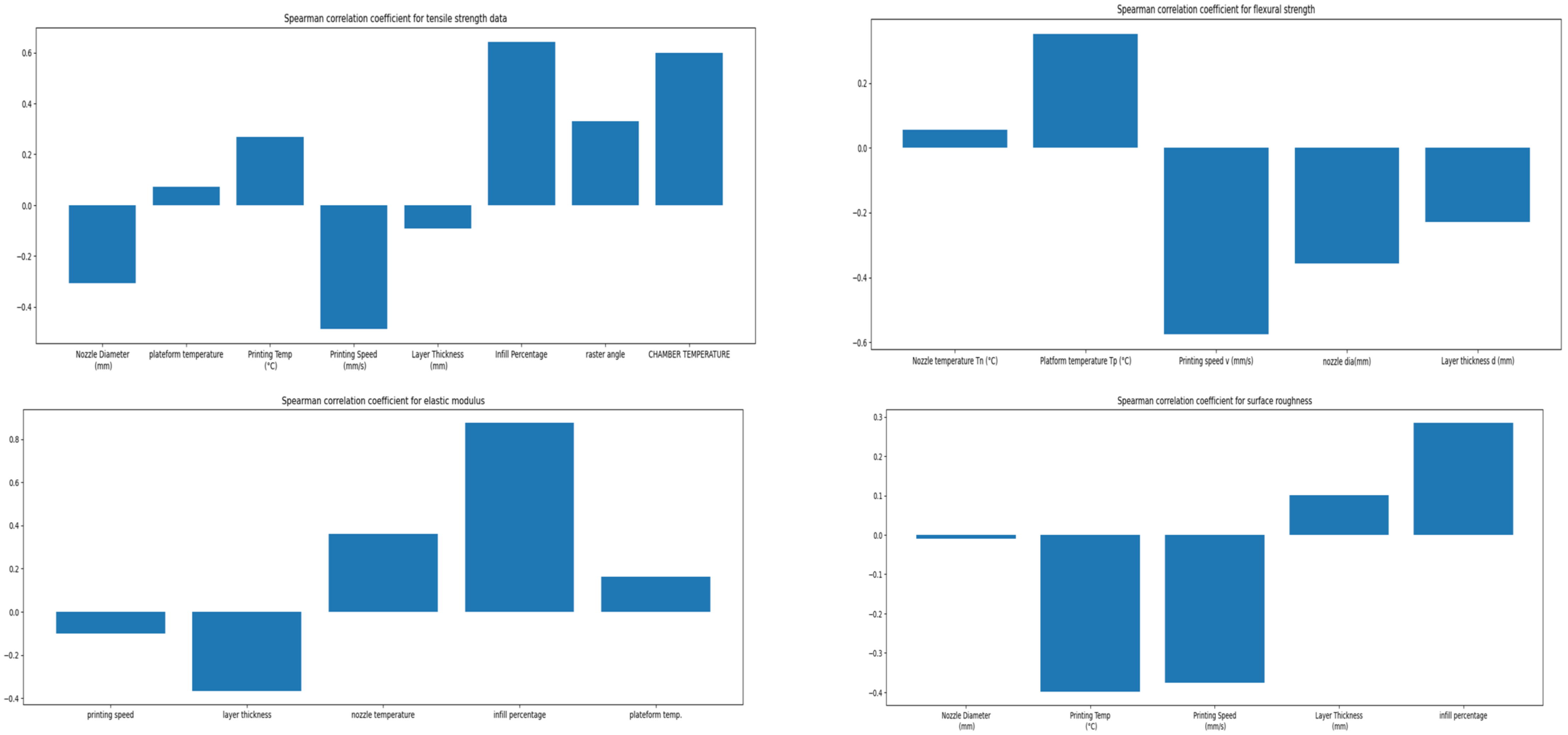

Fig 5: Spearman's correlation coefficient between target properties and process parameters.

ML models used for regression

Table 1: Mean squared error(MSE), Mean absolute error (MAE), Grid score for prediction of properties using various ML regression model is shown.

	Polynomial regression			Random forest regression			Support Vector regression			Artificial neural network	
Tensile strength	MSE		53.6	MSE		21.927	MSE		21.61	MSE	88.72
	MAE		6..3	MAE		3.32	MAE		3.54	MAE	8.17
	Grid Score		-1.2	Grid Score		0.7045	Grid Score		0.44	Grid Score	NA
Flexural strength	MSE		474.325	MSE		542.81	MSE		251.15	MSE	437.23
	MAE		18.06	MAE		23.179	MAE		13.59	MAE	17.52
	Grid Score		-0.056	Grid Score		-0.856	Grid Score		0.345	Grid Score	NA
Surface roughness	MSE		275.35	MSE		9.58	MSE		11.44	MSE	224.9
	MAE		14.73	MAE		2.44	MAE		2.54	MAE	12.7
	Grid Score		-0.18	Grid Score		-0.455	Grid Score		-0.783	Grid Score	NA
Elastic modulus	MSE		0.14125	MSE		0.0264	MSE		0.139	MSE	0.329
	MAE		0.358	MAE		0.136	MAE		0.353	MAE	0.553
	Grid Score		-9.2	Grid Score		0.52	Grid Score		0.086	Grid Score	NA
Combination of Tensile strength and Surface roughness	MSE	T	31.86	MSE	T	20.835	MSE	T	NA	MSE	21.50
		R	15.73		R	11.23		R	NA		
	MAE	T	3.3	MAE	T	3.54	MAE	T	NA	MAE	3.48
		R	4.5		R	2.78		R	NA		
	Grid Score		-0.3	Grid Score		0.16	Grid Score		NA	Grid Score	NA

Tensile strength	Flexural strength	Surface roughness	Elastic modulus	Combined tensile strength and surface roughness
None	Nozzle temperature and layer thickness	Nozzle diameter	None	Plate-form temperature and chamber temperature

Table 2: Process parameters dropped based on availability of dataset and correlation strength with the desired property.

Random forest regression	**Support vector regression**
- Ensemble technique that employs several decision tree to learn the dataset making it a low variance algorithm. - Each tree is trained on a randomly selected subset of features and uses a subset of the available data to make a prediction. - The final prediction is then made by averaging or voting the predictions of all the individual trees. - less sensitive to outliers, handles high dimensional data.	- It inputs data into a higher-dimensional feature space using a non-linear kernel function. - linear regression model is used to find the best-fit hyperplane that separates the data points into different classes. - hyperplane is chosen such that it maximizes the margin between the closest data points on either side of the hyperplane.

Table 3: Explanation of chosen ML regression model.

	Random forest regression					Support Vector Regression		
Hyperparameters	Max depth	Max features	Min samples leaf	Min samples split	n_estimators	regressor_C	regressor_gamma	regressor_kernel
Tensile strength	None	'auto'	1	2	100	NA	NA	NA
Flexural strength	NA	NA	NA	NA	NA	100	'scale'	'rbf'
Elastic modulus	50	'auto'	6	2	5	NA	NA	NA
Surface roughness	10	‘auto’	1	10	5	NA	NA	NA
Combined Tensile and roughness	30	'sqrt'	1	4	15	NA	NA	NA

Table 4: ML model chosen based on Mean squared error, Mean absolute error, grid scores, size, shape ,nature of the dataset and similarity in feature importance for the model with that of Spearman’s correlation bar plot. A k-Fold cross validation is employed to tune the hyperparameters for the chosen ML regression model.

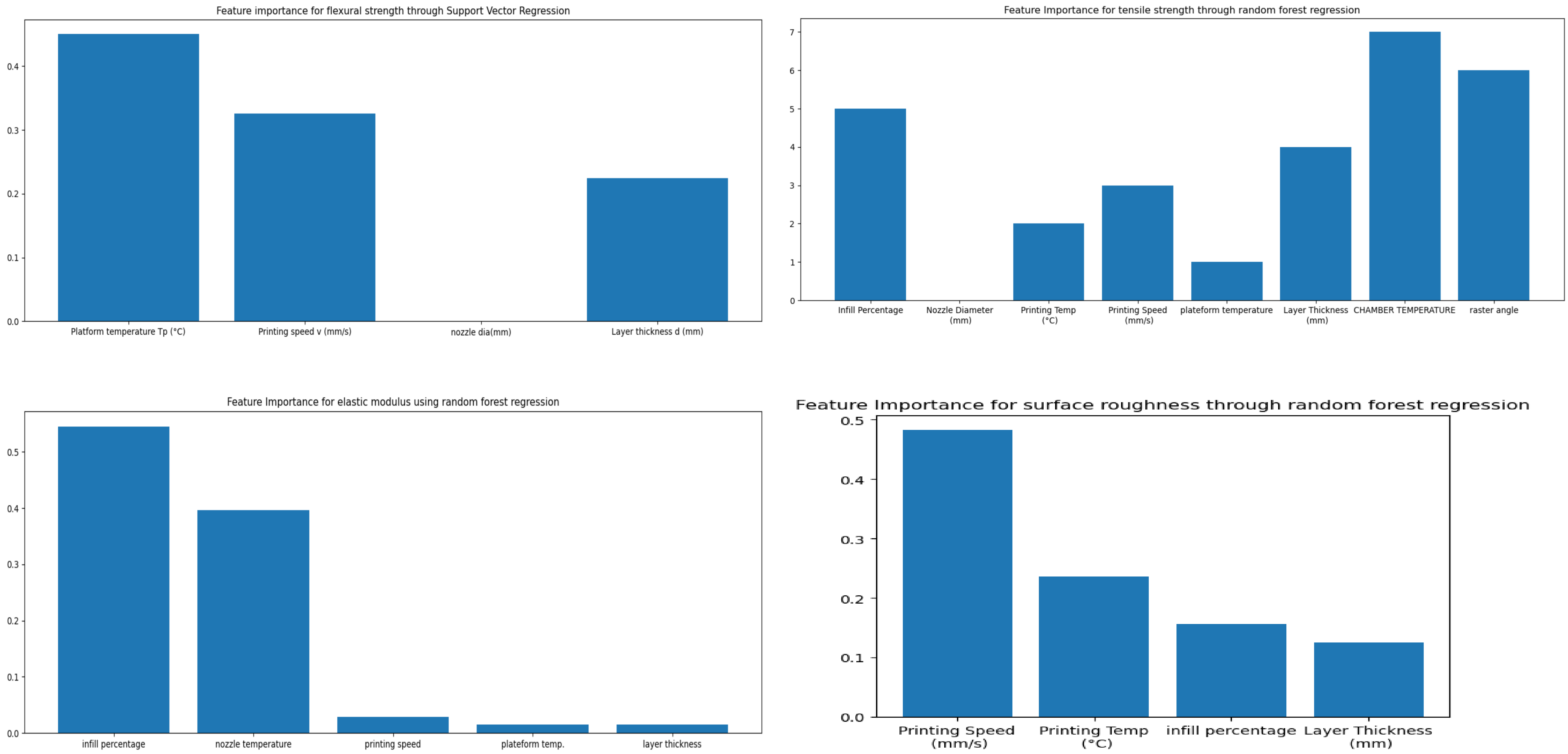

Fig 6: Feature importance based on ML Algorithm employed.

Interpretation of properties dependance on process parameters

Interpretation of tensile strength dependency on process parameters: [3]

- **Raster angle:** For printing direction perpendicular to plane of maximum tensile stress, layers are better in resisting separation.
- **Chamber temperature**: High chamber temperature results in low thermal gradient resulting in slower cooling of the printed part hence more time for crystallization and therefore better tensile strength.[4]
- **Infill density:** More material implies more resistance to loading.
- **Printing speed:** High printing speed results in improper bonding between layers causing low tensile strength.
- **Layer thickness:** Thicker the layer more will be thermal gradient across thickness resulting in higher residual stress and therefore less tensile strength. However, a very small layer thickness results in warping ,thus reducing strength.
- **Nozzle diameter**: Large nozzle diameter results in poor interlayer adhesion and more voids resulting in lower tensile strength.
- **Nozzle and plate-form temperature:** Higher temperature results in proper inter-layer bonding thus higher tensile strength.
- From the fig(1a-1e) , Outliers in data causes a higher MSE than MAE.
- Due to high dimensional data and small dataset[5] and there is mix of linear and non-linear relation between input and output dataset ,Random Forest Regression seems to perform better than another ML models.

Interpretation of elastic modulus dependency on process parameters: [3][7]

- **Raster angle:** This data was not used since for an isotropic material stiffness is not dependent on the printing orientation.
- **Layer height:** Thicker layer thickness can lead to a lower elastic modulus because it reduces the bonding between adjacent layers, resulting in weaker inter-layer adhesion.
- **Infill density:** More material will result in better connection between two layers thus providing more material resistance.
- **Printing speed:** Higher printing speed results in poor bonding and less crystallinity resulting in poor tensile strength.
- **Nozzle and plate-form temperature:** Higher temperature results in better bonding and increased degree of crystallinity thus greater tensile strength.
- From the fig(3a-3e)the , outliers in data causes a higher MSE than MAE.
- Due to presence of outliers[6], mix of a linear and non-linear relation between input and output dataset, high dimensional data and small dataset, Random Forest Regression performed better than other ML models.

Interpretation of flexural strength dependency on process parameters:[8]

- **Plate-form temperature:** Bed temperature determines how well the first layer of material adheres to the build plate. A higher bed temperature can result in bette adhesion and improved flexural strength. It also prevents delamination and warping.
- **Printing speed:** Higher printing speed can result in lower flexural strength due to decreased bonding between layers.
- **Nozzle temperature:** Usually a high nozzle temperature results in better bonding and therefore greater tensile strength but this parameter is not as important a plater-form temperature.
- **Layer height:** A smaller layer height leads to a smoother surface finish and better inter-layer adhesion, resulting in higher flexural strength.

Continued…..

- **Nozzle diameter:** Larger nozzles may deposit more material at a time, which can cause excess heat to build up and potentially warp or deform the part.
- From the fig(2a-2e), Outliers in data cause a higher MSE than MAE.
- Support vector regression performs better here than other ML models such as Random Forest Regression. It might be due to the fact that the dataset has a clear separation between the input features and the output variable. However, it still does not predict with good accuracy because other important process parameters like chamber temperature and infill density were not considered.

Interpretation of surface roughness dependency on process parameters:[9]

- **Printing speed**: A slower printing speed can result in a smoother surface finish.
- **Nozzle temperature**: Usually higher nozzle temperature results in smoother finish but when the temperature is too high, the filament can become too fluid and may not adhere well to the previous layer, resulting in a rough and uneven surface.
- **Layer thickness**: The trend in the fig 4d shows a trend which is counter intuitive and doesn’t agree with literature explored so far.
- **Infill density**: Increasing infill density should result in poor surface finish as the interior becomes more susceptible to warping, leading to poor surface finish.
- **Nozzle diameter**: Usually this is an important parameter for surface roughness however in the scatter plot and in Spearman’s correlation coefficient bar plot it is shown to be of less importance.
- Due to so many trends observed that are not in accordance with the literature, the best performing model Random Forest Regression gives a very high MSE and MAE as compared to average roughness value.[9][10]

<u>OPTIMIZATION METHOD</u> – **RSM(Response surface methodology)**

- The geometrical intuition behind Response Surface Methodology (RSM) is to approximate the response surface of a complex system using a mathematical model that relates the input variables to the response variable(s).
- The response surface is a three-dimensional plot that shows the relationship between the input variables and the response variable(s), where the height of the surface represents the value of the response variable(s).
- It then creates an objective function which is minimized or maximized using L-BFGS-B.
- The intuition behind L-BFGS-B is to find the minimum of an objective function by iteratively adjusting the parameters to minimize the function. At each iteration, the algorithm computes the gradient of the objective function with respect to the parameters, and then takes a step in the direction of the negative gradient. The step size is determined by a line search algorithm that finds the optimal step size that minimizes the objective function along the search direction.

Optimization of process parameters for optimal properties

Properties / Parameters	Nozzle temp. (°C)	Printing speed (mm/s)	Layer thickness (mm)	Nozzle diameter (mm)	Infill percentage (%)	Raster angle (degree)	Chamber temp. (°C)	Platform temp. (°C)	Optimal Property value
Tensile strength (MPa)	237.536	21.89	0.15	0.274	79.13	24.45	54.07	175.89	**47.9181**
Surface roughness (µm)	232.1	72.48	0.18	NA	86.67	NA	NA	NA	**14.89**
Elastic modulus (GPa)	264.42	12.868	0.153	NA	72.53	NA	NA	81	**2.64**
Combined Tensile and roughness	227.08	11.85	.18	.315	84.85	24.545	NA	NA	**66.42/13.2**

Table 5: Optimal properties for optimized process parameters.

Conclusion

- Random Forest Regression was used to analyze tensile strength, surface roughness, and elastic modulus, while Support Vector Regression was utilized for flexural strength.

- Response Surface Methodology (RSM) in conjunction with L-BFGS-B was applied to optimize the process parameters for achieving the desired properties.

- The optimization process aimed to optimize the values of tensile strength, surface roughness, elastic modulus, and combination of tensile strength and surface roughness.

- The optimized values of the properties were verified using the ML model employed for regression, and the results showed that the optimization process produced a nearly optimal solution.

Future scope

- More data is needed for better regression and optimization.
- More process parameters like printing pattern, chamber temperature etc needs to be explored.
- More robust optimization algorithm can be tried since RSM gives a near optimal solution.
- Incorporating microstructure of PEEK can give us a multiscale approach to optimizing process parameters.

Drive Link for Data and code
https://drive.google.com/drive/folders/1ThSTcxX3eB0OR5g_b1dhuCv1wJxA7JJV?usp=sharing

SOURCE FOR DATA COLLECTION

1. https://doi.org/10.1016/j.compstruct.2023.116901
2. https://doi.org/10.1016/j.applthermaleng.2019.114064
3. https://doi.org/10.3390/cryst11080995
4. https://doi.org/10.3390/polym13142344
5. https://doi.org/10.1177/09540083211009961
6. http://dx.doi.org/10.3390/ma11020216
7. https://doi.org/10.1016/j.cja.2020.05.040
8. https://doi.org/10.1080/2374068X.2021.1927651
9. https://doi.org/10.1016/j.jmapro.2022.11.057
10. https://doi.org/10.1002/app.49087
11. https://doi.org/10.1016/j.applthermaleng.2019.114064
12. https://doi.org/10.1016/j.polymertesting.2019.105948
13. https://doi.org/10.1016/j.polymertesting.2019.105948
14. http://dx.doi.org/10.1016/j.jmatprotec.2017.04.027

Reference

- [1] https://towardsdatascience.com/random-forest-regression-5f605132d19d
- [2]https://towardsdatascience.com/unlocking-the-true-power-of-support-vector-regression847fd123a4a0#:~:text=Support%20Vector%20Regression%20is%20a,the%20maximum%20number%20of%20points
- [3] https://doi.org/10.3390%2Fma15196801
- [4] http://dx.doi.org/10.1016/j.jmatprotec.2017.04.027
- [5] https://doi.org/10.1186/s12859-018-2264-5
- [6] Jump Start Your Modeling with Random Forests | Elder Research
- [7] http://dx.doi.org/10.3390/ma11020216
- [8] http://dx.doi.org/10.3233/ATDE220807
- [9] https://doi.org/10.1016/j.jmapro.2022.11.057
- [10] https://doi.org/10.1016/j.applthermaleng.2019.114064