**Advances in Additive Manufacturing of Materials: Current status and emerging opportunities**

**Prof. Bikramjit Basu**

**Materials Research Center, Indian Institute of Science, Bangalore**

**Lec47**

Welcome back to our discussion on emerging topics in additive manufacturing and what we are discussing before is the data science concepts like artificial machine learning and how they can be useful in predicting additive manufacturing outcomes or they can be useful in optimizing additive manufacturing process parameters. in the last lecture, I have started with the basic introduction to the artificial intelligence and machine learning. I am going to continue on the same topic in today's lecture. And while giving you some examples, I will also revisit what we learned in the last lecture. last lecture what we learned that overview of the artificial intelligence, then definition of machine learning and then how that is different from deep learning. one of the things that has been emphasized quite rigorously in the last lectures is that quality and quantum of datasets are very important.

Quality means there should not be any users biases in selecting the training dataset and test datasets as you know training to test dataset is almost like it is like 80 to 20 ratio like 80% training dataset 20% test datasets. And also we have learned that this machine learning or deep learning essentially depends on what is the quantum of datasets. For deep learning certainly you require much larger datasets than machine learning for example. And also that what we learned their performance of their algorithms of the machine learning or deep learning that enhances over time and that performance also improves over time and improves as they are exposed to more and more data sets in general.

what are the performance matrix that we have learnt? One of the performance matrix we learnt is that R square. R square is that is what we learnt in the basic mathematics and statistics. It is like correlation coefficient. And what you see this is the plot of Y versus X and all the combination of X and Y essentially are being shown. These are like discrete data points that will constitute the data sets.

But if you take a mean line which goes almost at the middle of these average data sets then what you can see then they are individual data essentially are dispersed almost at the equal side both on the upper side and lower side. And then how we can find out this R square value, R square value is essentially at any xi you have a yi value . how much this particular value of yi differs from the mean line value that actually determines how good

is that R square value. For example, what would happen if the R square value is just simply 1.0 that means all the data points should be perfectly lying on this particular mill line.

What will happen when R square is 0 that means that mean line would be somewhere flat and then all data points would be somewhere dispersed the way I just drew it. What would happen to R square value some random value 0.8, 0.9 then there will be some data points will be essentially dispersed at some lengths from this mean line. it all depends on so, if the R square value is 0.

99, then what would be your guess? Your guess would be that these particular data points will be now extremely close to this particular average line. the higher the value of R square closer to 1. Then these particular data points in a given data sets will be essentially lying very close to that particular trend line or mean line or average line. R square although I have mentioned correlation coefficient, it is also known as the coefficient of determination. It is essentially 1minus RSS by TSS.

RSS is the sum of the squares of the residuals. what is the sum of the square of the residuals that is yi-yi cap hat values, value square. And then TSS essentially means the total sum of squares, so this is one of the performance matrix. Another performance matrix is the root mean square error, so root mean square error is 1 by n sigma is equal to 1 to n yi-yi cap hat square and then your R square value should be close to 1 and your RMSE value should be close to 0.

0. this should be close to 0.0 and this should be R square value should be close to 1.0. the residual error if you plot it that should be Gaussian in nature. The maximum probability density should be lying around the origin that is 0.

0. what you see the probability density of the residual error you can see this is for the training dataset and this is for the test dataset. training data set is 80% and test data set is 20%. you can accordingly see that bar heights and all those things are also much lower, therefore just to summarize that what are the performance matrices. performance matrices is orange line essentially difference between the observed and prediction and residuals calculated for both training and test data sets. good residual plot I have mentioned.

this is the 3 points. first conditions is that R square close to 1, RMSE close to 0 and third one is a good residual plot that is a high density of points close to origin and symmetric about the origin. Now, machine learning essentially uses two types of algorithm. one is called regression and one is called classification. Each of them have their own significance, regression and classification.

what is classification? Machine learning task that deals with identifying the class to which a predicted output belongs. And often this predicted output may not be some numerical number but some quality related labels for example. a classifier is used to distinguish two or many levels for example if you give the test insistence and they have some attributes A1, A2, A3 and classifier essentially will result in giving discrete valued class level here Then one of the example that I just I mentioned for example in the context of 3D printing or laser based 3D printing you have a laser power, you have a scan speed and you have a powder feed rate and you have overlap. Powder feed rate like for example this is the case for the DED directed energy deposition case. what will happen if you give all this data into the classifier, classifier will essentially generate two levels.

That one level will indicate that the component that you are fabricating using a specific combination of these processing parameters will have a defect, yes or no. And if you further level what kind of defects you can give some classifier value then you can say that what kind of defect one can essentially predict. performance matrix in classification that is something called confusion matrix. confusion matrix essentially you can have a true negative and false positive. it is between binary 0 and 1, 0 prediction and 1.

actual is 0 and 1 and prediction using the classifier task what you can predict 0 by 1. if it is matching 0 0 that means it is a true negative prediction. If it is 1 and 0, then it is a false negative. If it is a true positive, that means it should be 1, 1.

This is 1, this is 1. And then if it is false in the quadrant of 0 and then 1, then it is called false positive. for example, it is being shown here in a confusion matrix, there is a true negative is 14, false positive is 13, false negative is 2 and true positive is 1. here you see that some of these emails that has come. there is either no spam or there is a 1 is a spam. in the spam case you will see that is a 3, 1, 2, 3, 3 is the spam that is false positive and true positive is only 1 that is a correct prediction is true positive is 1.

if you look at this confusion matrix here actual versus prediction then you have a true negative, false negative, false positive, true positive that kind of combinations you can get. accuracy is essentially what is the number of correct predictions and what is the total number of predictions. typically true negative plus true positive divided by sum of all. that is the what is the accuracy of the predictions in the classification task. it is here it is 75% is the accuracy.

Precision, precision is the true positives divided by true positive plus false positive for example. here you can see that what is the true positive. What is the true positive is 1 and what is the true positive is 1 and false positive is 3. 1 by 4 is 25% is precision. what are the parameters? What is the parameters that we are learning from this discussion is that

classification you have to learn one is the confusion matrix, Second one we learn what is the accuracy.

and third one we learnt that is what is the precision. this accuracy in precision it is depends on actually the combination of true positive, true negative and false positive and false negative . that we have learnt. Now recall, recall is the another one and recall essentially defined as true positives divided by true positive plus false negatives,   that is a recall and recall here in this particular case that we discussed in the context of the spam and non-spam emails is 33%,  essentially what you see here that in one end you have high precision, low recall and another end you will have low precision and then high recall.   let us substantiate    what    we    are    trying    to    do    using    that    classification.

this is just a like overview. what you see here? This schematic essentially shows the input parameters of directed energy deposition of titanium 6, aluminum 4, vanadium. This is the materials which has been very widely investigated for aerospace to biomedical to various other structural applications. Now, what are the parameters of importance is laser power, scan speed, powder feed rate and overlap in case of multitracks. Overlap means suppose you    have    one    track,    you    have    another    track.

this is a third track.  while scanning this kind of track, the way I am describing that what is the overlapping percentage between the two adjacent tracks. there are different type of defects that normally are observed and recorded in the directed energy deposition. One is a lack of fusion. You can see that there is this particular area if you look at.  this is kind of you    know    falling    off.

Then there is another one called intertrack porosity. Do you see very closely if you look at this particular area, these are called intertrack porosity. that means melting and solidification did not take place very very precisely leading to this intertrack porosity. Third one is the green one, green boxed one and you can see this particular Ti6Al4b this is absolutely defect free like there is no lack of fusion and neither any intratrack porosity. those are the 2 defects and there is perfect conduction has taken place and that is called this conduction.

we have generated very small datasets and every time as I mentioned that in the AI-ML approaches you have to essentially mention that what is the quantum of datasets. it is 56 datasets. Out of these 56 datasets, you have the positives, negatives, true positive, true negative, false positives, false negative and true negatives. And then if you see that positive versus positive is Tp, negative versus negative is Tn. And then you can see that  these are the things, output values that will generate and then what we learn, this is as a confusion matrix.

And when you do that subsequently what you learn from the previous slides then you can essentially calculate what is the accuracy, what is the precision and what is the recall value. These 3 values you can clearly mention when you are handling in a particular data sets. in terms of the melt pool geometry, this is more on a regression based analysis. as I said that two things are very different, regression and classification. And the regression based analysis again laser power, scan speed and powder feed rate, these are the inputs.

then output is your what is the melt pool width, depth, height and area that is single track. And then you essentially assign some models. And then we have generated let us say 96 data points and then we have k cross fold validation, so here the k value is 5, what we learnt as the k cross fold validation, here k value is 5. And then we have used different type of models, ML models like linear regression, Gaussian process regression, AutoML, gradient boosting machines and so on. unsupervised learning that essentially reveals patterns within data.

that we have mentioned before, you know, when I started this lectures on the concepts of data science. then group and interpret data based on only on the input data. there can be couple of observations. One can be clustering of data. it can be clustering, one can be generative adversarial networks, then variational autoencoders, normalizing flows and diffusion                                                              models.

These are the three things that we have learnt. these are the things that we are not going to discuss in too much details like you know GAN for example, general adversarial networks and so on. what we are going to discuss more in this particular lecture as well as the next lecture is a machine learning pipeline in practice. creating a fingerprint of your material, this I have mentioned for example, same material, similar compositions but you know some of the addition to these materials is different. For example, if you are not using the standard titanium 6 and 4 vanadium, use a titanium  X aluminum and Y vanadium and then you are using          the          different          values          of          X          and          Y.

So, essentially this material value will be one combination X and Y, material 2 can be another material can be different combination of X and Y. Depending on what is the combination of X and Y, you can essentially measure the properties P1 to Pn and then material 1 related to P1, material 2 related to P2, material related to Pn and this is the fingerprint. that you generate when you try to establish P, essentially PSP, so process structure property correlation, that kind of correlation. what is fingerprint? Fingerprint is a unique numerical representation of a material. this is a fingerprint like F11 and F12 these are like fingerprint and a condensed signature of material easy to compute and has a physical     and     chemical     relationship     with     the     property     to     be     predicted.

these are certain things that you need to develop. these are like fingerprints is more like a descriptors. what are the descriptors that will essentially determine the properties. Now in the context of metallic materials many times grain size can be one such descriptors because grain size essentially influences the properties like hardness or strength for example. Now step 4 is that selecting a machine learning algorithms then as I said that you have to use different type of algorithms because you have to see what is the combination of R square, RMSE and residual error.

residual error curve. these 3 combinations will not be optimized the way we want them for any given ML algorithms whether it is a polynomial regression or whether it is ANN or whether it is GPR that is also very useful that is Gaussian process regression. Then as I said step 5 would be entire datasets  you essentially segregate in 80 to 20 ratio, 80 is your train data set, 20 is your test data sets and then that should be done in a very unbiased manner. Then, optimize the model complexity bias versus variance trade-off and then need the model to be complex enough without being overly complex and cause overfitting. And then step 7, test the accuracy of the model like you need to have some validation datasets. Using the validation datasets, you can essentially test the accuracy of the model.

there are some couple of case study that I am going to show you before the end of this specific lecture. This one of the things is that patient specific dental implant, Now these dental implants is also being shown in this particular NPTEL course I am giving  some of the basic concept of dental implants, what are the metallic dental implants, ceramic dental implants and how 3D printing can be used to manufacture dental implants, those concepts, those examples are being taught. Now, here what you see patient specific dental implants which is a very rare cases like in a mostly dental implants are varied in different sizes like for example, 3.7 mm diameter can be 10 or 12 mm length for example, using finite element analysis and computational intelligence techniques.  you have a model and they have a assembly of natural molar teeth  And this assembly of natural molar teeth, if you see that it can be either solid implant or can be porous implant or dental implant with mandibles.

In all these cases, you can do this, what is the finite element analysis, FEA, trying to see that in case of these dental implants, if it is placed in the molar region of the jawbone, that what would be the stresses and strains that will be generated. And then one group based in India, they have done this analysis, they have used that artificial neural network and then they have used this artificial neural network and particularly genetic algorithm that is a population candidate solutions to an optimization problem has evolved towards better solutions.  this ANN and particularly GA technique were used for  the better designing of this dental implants,   you have input parameters and you have output parameters and these are like hidden,  Case study 2 that is machine learning technique for the optimization of

joint replacements, this is like short stem hip implant. short stem hip implant for example in the context of total hip joint replacements one of the newer concept is to use the short stem. that means the length of the stem is shorter and accordingly other parameters stem width and the way it is being, it gets reduced in cross section from top to bottom, those thing needs to be optimized.

that is the case for the femur model, geometry and material properties assignment and here these particular studies like Cilia et al which is published in PLOS One, they have taken the different parameters like L, D, R1, and R2. this L, D, R1 and R2 has been defined here. L is this total this length, D is this particular specific length and often this particular specific length is coated with hydroxyapatite whether it is the case for the titanium implants or stainless steel implants. Now, if you look at the medial, posterior, lateral and anterior, so these are the two different radius, these are being mentioned here, one is R1 and one is R2. And these L, D, R1, R2 are the four different parameters and you know in terms of the material assignment, you can get this radio density like Hounsfield unit, you can get the apparent density, you can get the elastic modulus E.

So this is like for sampling purpose and for segmentation purpose and thresholding, bone and soft tissue, these are the different things. here in the machine learning models, they have given the input parameters L,D, R1, R2 and output is the mean of the differences between the implanted and healthy femurs in the areas of the study. So, in case of the healthy femurs, what will be the strain normally it is generated. In case of the implanted femurs, what is the strain that is predicted to be generated. Case study 3, this is the machine learning approach to estimate stress distribution as a first and surrogate, effective surrogate for the finite element analysis.

what are the things that you see here? You can see here that this is the aorta. Through this aorta, blood is transported. Now this aorta, one of the main things is that aorta shape as the input factor because that is very important and what is the wall stress distribution. When blood flows through this aorta, what is the stresses that will be generated in the aorta wall because that stress will have an impact on the cell fate processes or that many times in the tissue maturation. what they have done they have essentially this particular work is done by Chinese group Liang et al and then what you see here they published in journal for Royal Society of Interfaces in 2018 they have essentially used different functions here.

and different parameters and they have used certain data sets for example 256 data sets and they have essentially used the shape parameters, input parameters and output parameter is the stress. if the shape parameters change then the stress parameters also will change. And therefore, their input is shape code and output is a stress code. directed energy deposition in the laser based process, high energy laser beam is being focused and where

powders is being impinged. When you make this complex shaped large components like this is a relatively simpler shaped here, but it is large components.

Then, it is expected that when this part is being manufactured, large shaped manufactured and this laser beam which is focused on that, there is some distortion of the parts because of the either high scan speed or the combination of high laser power and scan speed. A is your fabricated disc. B is your distortion and distortion if you see along this scale is micrometer micron, along this scale is millimeter scale, other scale is a millimeter. you can see this dotted one, you can see this is bent, this part is negative distortion, this part is positive distortion with respect to the original shape of this component. what you can see here that with more and more temperature, more number of layers are being fabricated, For example, you can see here is a laser power and scan speed, you can also see that so many different kind of components are being manufactured and this is the actual powders which are being manufactured as a raw materials, you give all those things and you apply the deep learning model, then deep learning model allows you to predict that for a given combination of this laser beam power as well as the scan speed and powder feed rate, what is the shape predictions or shape distortion that it can happen using the directed energy deposition.

I stop here and then I will continue in the next lecture on this introduction to AI-ML. Thank you.