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

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we start with this another scientific case study and this time this scientific case study will be on the regression analysis. of the DED directed energy deposition mediated 3D printing. some of the fundamentals that we learned from other AI-ML approaches, this is the basic workflow. -let us recapitulate what we learned because these are the things many material scientists or people in that bioengineering discipline are still not using. I know that some of these slides may be repetitive from the last three lectures here as well, but I think it is instructive to show this kind of very important fundamental slides for you to realize that how this machine learning as a field can be very useful to the overall technology of the additive manufacturing. you have a raw data sets and then you have a cleaning dimensional reduction and extraction.

then you have get features and output these particular things that you must be now, you must be knowing it by heart that you have a training datasets and you have a testing datasets, training is 80%, testing is 20% and testing often also includes validating sets. you start train the datasets, this 80% unbiased or randomly selected datasets of the overall 100% datasets. in this particular case, if you use different type of models and these different models are giving as an input to the machine learning workspace here, where hyperparameter selection and validation process will be operated. then what we get essentially that what is the performance of difference models.

this performance essentially is measured by three matrices, one is that R square, one is RMSE and one is the residual error analysis. these three particular metrics that received by these three particular metrics that you know we use for this performance value for the performance metric analysis of the different machine learning models. And once we finalize one specific model for this particular given training datasets, then what we use for you, we can tune this particular model for this using the validation datasets and then we can also do that estimate and predict for the particular using the testing datasets. all these exercises that dotted arrow essentially will give rise to final model that this final model will give rise to some empirical relationship based on for example, what we learnt in from the earlier example GPR. or GBM, Gaussian process regression or gradient boosting machines.

that gives you the predictions and this prediction is statistically most reliable if and only if we use the critical quantum of high quality datasets as an input to this entire workspace here. I think this point I have been emphasizing time and again in the last three lectures and I thought that it will be, it is instructive to again re-emphasize here again once more. The another concept that we have also shown that is K fold cross validation and in one of the cases I have mentioned earlier that value of

K is 5. So it is essentially cross validation means you are validating and you are again cross validating. you have a original datasets, you have a test datasets 20%, training datasets 80%.

 what you see that what is the training folds here? and what is that MAC values that also we have mentioned before. you have these training folds. And then what is that MAC values and here you can see that what is the best hyperparameter combination for ML models like KNN, K nearest neighbor, support vector machine, artificial neural network, decision tree, random forest, gradient boosting machine, GBM. you get the best models, then you predict using the testing datasets, then your predictions and then you find out that what is the final matrix. But you can also show this fitting the dataset, fitting the model that is the best, that is always done using the training datasets.

 this is like what is the notation that is used in machine learning model. model is always described as y is equal to f of x square bracket x, where x is the input that is variables always Roman letters, output is y that is normal is scalar, bold is vector and capital bold is matrix. this one of the things that you also learnt earlier that is the loss function and this loss function needs to be maximized. loss function or cost function in the machine learning language often they are essentially denote how bad a model is. and how bad a model is that is kind of described by loss function L phi.

 it returns a scalar that is smaller when the model maps inputs to outputs better. the smaller the value of L phi the better is the performance of the model. loss function is the difference between models prediction and actual values and training objective is to minimize loss function. all the places that you have seen that your training data sets that essentially train the machine learning model and this training model and models predictions using the test data sets and actual value. The smaller the difference, better is the performance and smaller the difference means that L5 value is also   minimized.

 loss function value is to be minimized. this is to be minimized,   what is regression? Now I mentioned before there is two type of basic task, one is a regression and one is classification. Regression is a statistical model which estimates the relationship between the dependent variables and one or more independent variables. And input parameters here for example in case of regression, let us say laser power, scan speed, energy density, powder feed rate. this 300, 720, 25, 5 these are like arbitrary set of values of this input parameter that will constitute the matrix of the model input which will be essentially trained using the let us say one of the supervised training model   and   this   is   the   model   output.

 And this predicted output you can predict that what would be the track width for example is 78.34, these are random values just for the illustrative purpose. And for example from experimentally measured values is 84.31 and your predicted width is 78.34, so it is almost like 10 micron off from the actual values, essentially this regression models can be classified to univariate regression and multivariate regression problems like one output real value, multiple outputs real value.

 one of the common models that were used by many times these researchers in the linear regression model and there they use the mean squared error as a cost function. You remember that you know few slides back you have seen that original datasets can be classified or can be segregated into very

randomly in an unbiased manner training datasets and test datasets. And this mean squared error is MAC1, MAC2 for example this is a different training faults and these are like mean squared error this is like a cost function or L phi and this L phi needs to be minimized in this particular case. Now, here you have the data points, random data points and this particular 45 degree line is called line of regression and the y is your dependent variable and x is your independent variable. I recall at the beginning of the artificial machine learning, I have mentioned to categorically that AI-ML is most effective when there is no established empirical relationship between the output and input variables or that means dependent and independent variables in those kind of cases AI-ML plays an   important   role.

So this is the gradient descent that is used to minimize the mean square error or loss function and it also uses the gradient descent to update linear coefficients by reducing the cost function that you have mentioned. And this cost function as you see it goes from 0, 1, 2, 3, 4 and you can see accordingly output and input functions that also changes or it also varies. here y is equal to mx plus c, here y is equal to a_0 plus a_1x plus epsilon, epsilon is your random error, a_1 is your linear regression coefficients and a_0 is your line intercept or in that y-axis intercept, Performance matrix have been told multiple times, so I will just go through very very first and this particular box I would like to highlight because this is the thing that you all need to remember. Your R square value should be close to 1, your RMSE value close to 0 and good residual error plot should have a high density of points close to origin and it should be symmetric about origin. what is classification? regression I have mentioned, classification I have mentioned before and I want to mention it again.

That is a machine learning task that identifies the class to which a predicted output belongs. And many times this predicted output, this classifier is used to distinguish two or more levels. For example, your test instances are different attributes a_1, a_2 till a_n. you have to find out what is the discrete valued and class level. Another example in the context of additive manufacturing, for example, you have a laser power, scan speed, powder feed rate overlap you would like to know whether a specific combination of AM parameters will result in defects or no defects.

And here you can see that the classification algorithm allows you to predict that whether a particular combination of parameters will result in defects in the parts or not. there are certain things that I have mentioned you before in the classification 1, you have a confusion matrix and confusion matrix essentially will be a description or will be a plot between the true or actual class versus predicted class. And true or actual class here it is a true and false and this is a positive and negative. there is something called true positive TP, false positive FP, false negative FN and true negative TN.   you   have   some   cases   is   true   and   some   cases   is   false.

positive means true positive plus false negative, negative means false positive plus true negative. false positive means it should be negative and true negative is already negative. Similarly, positive means TP means true positive and false negative. there are other parameters that we have mentioned.   This   confusion   matrix   is   one   thing.

Other parameters that we have mentioned is the precision. Precision is true positive divided by true positive plus false positive. Recall is true positive divided by true positive plus false negative.

And third one is accuracy. Accuracy is true positive, true negative.

They are additive values divided by the sum total of all other values that are used to describe this particular matrix. And then other one, F1 score is essentially 2 multiplied by precision into recall divided by precision plus recall. what are the things you learn? One is the confusion matrix. One is precision. One is accuracy, one is recall, and fourth one is F1 score, the other things that if you plot true positive value against false positive value, then if you get this dotted line, this is called random classifier.

And this random classifier, if you go on the off side, it will be worse. If you go on the other side, it will be better. this is called ROC curve, that is receiver operating characteristic curve. one end you can see is a perfect classifier. like 1 value the true positive when it is 1.

as it goes from the random classifier value towards the left hand side that your prediction of the classification algorithm improves and area under the curve A you see , If it is 1.0 then ROC is perfect. ROC is perfect means this 1.0 this line the way I am drawing the same line is been drawn here.

If AUC is 0.5 area under the curve is 0.5 then it is the half of this area so that means this is the hatched area here and ROC is the random. interpretability in the black box ML models, so ML models often is being criticized because we do not know what is happening inside the ML model and why this specific ML model performs over another ML model in terms of the quantitative performance matrix. whenever you are quantifying certain thing as a scientist, we believe that particular aspect, But the question is what is the basis or what is the rationale of our trust or belief on the ML models when we do not know what is the different equations that are being generated to fit the model better and better. one of the values that is often used is called Shapley values, S H A P.

that is essentially for interpretable ML models. based on cooperative game theory, so many if you look at the history, so game theory is one of the aspects that game theory is one of the theories that actually accelerated the development of this total artificial intelligence field in the early stage. Shapley values is a model agnostic method for explaining machine learning predictions and it reveals how each feature contributes to the final output. what is the SHAP surrogate model? For example, here g z prime is a local surrogate model of the original model fx and this is phi i is the contribution of feature i to the final output. what you see here? This is your input, this is your black box and this is your output.

SHAP is essentially applies to see that how this Shapley values is a model. you have the data, you have a model and model gives your Shapley values and you have a prediction and Shapley values are used for the explanation of the model predictions. there is some more example like more mathematical description of what we have discussed like marginal contribution calculations like this is some of the functions that are used for this marginal contribution calculation functions here. Now, in the particular case like when you use a combination of laser power, scan speed and powder feed rate, now you want to predict that what will be the clad width for example or somebody is

interested to know what will be the clad depth for example. what is the algorithm? Algorithm is the calculate all possible permutations.

For each permutation take the set of features preceding our target feature. Third one include the target feature in the subset. Fourth one subtract the contribution of the subset excluding the target feature. Now this is the different values.

P is power. SS is scan speed, PFR is a powder feed rate. Let us say value of power is Vp is 10, powder feed rate is 9, 8, 27, so P plus SS, so then it would be 27 or Vp plus power plus PFR powder feed rate, it is 35 and so on. then if you see that what is the order of R, like P, PFR, power, powder feed rate and SS scan speed, the contribution Vp is 10. PFR contribution is V of PFR, P minus V PFR, so it is coming out to be 36. that is powder feed rate contribution and scan speed contribution is 10.

on the basis of this simple mathematical calculations, you can essentially see the different features like P, PFR SS, what was the initial value that is 10,9,8 and what is the payout is 17.5, 16.2 and 11.5 that is the SHAP value. Although scan speed is 20% less because scan speed is 20% lesser than power like 10 is the power and scan speed is 20% lesser.

It contributed 34% less than power and powder feed rate contribution is even much closer to power. what I am saying from the values here 10 versus 9, you can say it is 10% lower. But the relative contribution of powder feed rate is very close to that of the power although their difference in values is only 10%. Now, with respect to power if you see the scan speed is 20% lower here in this original contribution. But based on the Shapley that their relative contribution is 34% lower than compared to the laser power.

that is what has been mentioned here. this is like payout is 17.5, powder feed rate is 11.5 and scan speed rate scan speed is 16.2. Let us move on to the some of the examples of the DED 3D printing.

As I mentioned that you know that in case of this DED 3D printing, you can see that there is some of the examples that I have given the dilution, this is the depth and this is the height. here dilution is 0. depth is 0. depth is 0 and capital D is your dilution. This is the height and this is the height and depth.

there is a 2 things. Here H is greater than D and here H is less than D and here H is 0. A is the case for the lack of fusion, there is absolutely no fusion of the substrate. B is the case for the optimum dilution and C is the case for key-holing, like when depth is very large, then there is a key-holing type of defects that can result from that combination of this one. I repeat H is 0 is the perfect example of the lack of fusion defect, H is much less than D that is the case for key-holing, H is greater than D that is the optimum dilution. if you have the clad bead area that is Au, you have a penetration area as Al and you have the other parameters like W, then there is a H parameter and h is the track height and then your d is the track width your d is the track penetration depth.

Now, in case of overlapping things that as I said that what is the dilution and overlapping. 2D cross

section of your single track. This is the 2D cross section of your neighboring single track. what you can see between this and this, this is the overlapping area like the way I am circling. Between this track and this track, this is the overlapping area because this is the common area which belongs to both the tracks, this is the overlapping area and there you can see that what is the overlapping valley and so on and from there you can calculate what is the overlap percentage, w-dx by w into 100, dx is your hatch spacing.

capital Dx subscript x is your hatch spacing, hatch spacing is essentially the distance between the two maxima point in your height of this single track. that is your hatch spacing and W is capital W is your width essentially and the width of the multi-track. this is the complete width of the multi-track from here to here. This is the complete width of the multi-track divided by W into 100. on the other materials like titanium 6, aluminum 4, vanadium, earlier in one of the earlier lectures I have shown the regression study of stainless steel 316.

You can see depending on the materials, depending on the combination of parameters that we use to generate the complete datasets and also quantum of datasets that you can see that you know how the different combination of parameters are used to generate this single track. So you can see on the same plate how many large number of single track. single track titanium 6, aluminum 4, vanadium material were deposited and then what you see that you get essentially Au, Al, capital H, small d and W that is the track width. this is the range of power that were used. This was the range of scanning speed that were used and this is the powder feed rate.

total is that 240 datasets are generated and the 240 datasets first we have done is the Pearson correlation coefficient and then Pearson correlation coefficient were very useful to find out that what is the PCC correlation coefficient essentially shows the relationship between the melt pool parameters and the process parameters here input is power, scan speed, energy density, powder feed rate. Output is all the track geometry parameters, single track geometry parameters. So different hyperparameters. which are studied in machine learning models for all the task is the linear regression, ridge, lasso is alpha you know their values is 0.

001 to 100 these different ranges are also studied. And then subsequently these different other CAD boost and MLP multi layer perception models were used Gaussian process regression GPR and gradient boosting method GBM and light GBM. now if you see that what is the regression matrix on test data sets of the explored ML models, depth, width, height, penetration area and clad area and you can see that for different things your R-square value is very high for the decision tree and random forest. In the case of width also R square value is high, in case of height also R square value is very high close to 0.8 or so and clad area is also R square value is quite high around 0.

9. Now if you see that for example GBM the gradient boosting regression model. here with SHAP interpretation, what is SHAP? I have already explained to you before. With the SHAP interpretation, this dotted line is your ideal line. training and test data sets, these are like distributed very, very close to this dotted line. this is the true value and this is the predicted value and this is your shap value that impact on the model output.

And you can see this particular scan speed has that maximum impact that means shap value is 0.14. Whereas power has the shap value of 0.

10, 0.10, energy density is 0.03 and powder feed rate is very, very less. So scan speed has the maximum impact on the predicted output value. The residual error that I have mentioned before that it should have Gaussian type of distribution and exactly if you see the large probability density, maximum probability density is 001 and this is the case for the Gaussian type of distribution for both training and test data sets. Now gradient boosting regression in case of width also we have seen that similar kind of distributions. You can see this dotted line is the ideal line of regression and this all the training and test data sets are actually dispersed very very close to that line of regression meaning the RMSC value must be close to 1 or close to 0.

0 respectively. Here again scan speed the impact of scan speed is much higher 0.08 compared to other parameters like power and so on. same is true but the case for the depth, it is the different kind of regression models that we have used and that gives us more confidence on the performance matrix that is called XGBoost. In case of XGBoost, it says that testing and training datasets, these are actually dispersed very close. One of the important thing that we have found out in case of depth and that is quite arguably correct is that the power has much more impact as per the shap analysis compared to scan speed.

In earlier cases, scan speed is important, but here power is much more, so it is 0.09 for example. compared to the scan speed, so that is very clear and in case of R square value it is 0.999 that is for the training data set, for the testing data set is 0.

936 and RMS table is 0.004 or 0.038 is reasonably close to 0 or very low. clad area is again gradient boosting. except the depth it is all are gradient boosting and here again like similar to earlier cases you can very clearly see that is a clad area is also training datasets. This is essentially very much Gaussian distribution as well as the testing datasets. scan speed does have strong impact on the output magnitude here.

Now in case of the penetration area, it is a cat-boost regression model. Penetration area is like this particular area here. Penetration area it is a cad-boost model and you remember XGBoost actually for the same datasets was performing better for the predicting of the value of D that is the depth of the weld pool or clad pool. And here again another different algorithm or CAD boost regression model with SHAP interpretation that actually was very much useful for predicting the penetration area. like depth penetration area also you can see that is the power has more impact compared to power has more impact as analyzed by SHAP compared to the scan speed. this is the summary of the model performances like gradient boosting, AXG boost, gradient boosting, gradient boosting and CAD boost.

height, width and clad area, these three are gradient boosting, XGBOOT is most for depth of melt pool and penetration area is more for clad boost. in all these cases if you see R-square, RMSC values are very very close to 1 or 0.0 and that is what it should be for the best performing models and we have also seen that statistical distribution of this residual error that follows more like a

Gaussian distribution with the maxima near 0, 0 that is the origin. this is the summary, you have the input parameters, DED process parameters, laser power, scan speed, powder feed rate, your melt pool geometry is a generated data set is 240 like track width, track height and penetration depth and what we have shown the different models that essentially gives rise to RMSE and R square score very close to that of the statistical acceptable values as we have seen and then SHAP interpretation was very useful to determine the relative impact of the input parameters on the predicted output. That has been shown while showing individual predictions of the track width or track height or penetration depth or penetration area or clad area as I have been discussing for last 10   minutes   or   more.

 Now next few minutes. Before I close this lecture, I will be showing you some results, some of the case studies of our unpublished results on the direct energy deposition 3D printing for the classification. If we recall that our earlier discussion that classification is one of the machine learning task which is used to identify that whether specific type of defects. will be generated for a specific combination of additive manufacturing parameters. And here you have used for single layer multitrack experiments let us say different power has been varied, scan speed has been varied, powder feed rate has been varied and hatch pattern also is mostly simple zigzag pattern. And we have mentioned the code like HS7 for essentially overlap is 0 and go up to 66% overlap if you go to   HS4   for   example   66%   overlap.

 And what is the overlap? That I have discussed a few minutes back. Overlap is essentially calculated by the area of the overlap. area of the overlap or which is the area which is common between the two adjacent tracks in the multi-track experiments. just a combination of different parameters like 350 watt laser power, 360 millimeter per minute scan speed. Now, if you increase the overlap, now whenever you see that is the green colored one box, that means this is the perfect conduction   without   any   defect.

 That is what I am mentioning here, no defect. That is the case for conduction. these particular no defect cases are valid at the essentially this particular area of this map that is 350 watts and also 400 or 450 watts, 480 millimeter per minute or 540 millimeter per minute. All these red ones are essentially intratrack porosity like you can see, intratrack porosity. Yellow ones is the lack of fusion, there is no depth, there is lack of fusion. lack of fusion is certainly not acceptable in a industrial sector or in a commercial sense. We need to have this kind of green ones that is the defects,   there   is   no   defects   and   this   is   a   perfect   conduction   case.

  we need to have this kind of green boxes, where there is a perfect conduction multi-track weld that has been generated particularly in case of Ti6Al4V. this is the dotted ones which shows that what is the distribution of the conduction cases as a function of different combination of the process parameters. Now logistic regression based defect detection classification. So you remember the test confusion   matrix.

  test confusion matrix and train confusion matrix. Here again in the classification task you have to randomly segregate training set, data set and testing data sets the way we have mentioned like 80 to 20 ratio. therefore if you count 26 plus 1, 27 for 3144, 44 is this your data sets in the training and

in your test it is 12. 44 is almost like 80% and 12 is almost like 20% is of the data sets, you have that actual and predicted. you have a true positive is 26, true negative is 13, And from this true positive and true negative, what are the things you learnt earlier? You can essentially calculate, this is your confusion matrix. You can essentially calculate what is the precision, what is the accuracy, what is the recall and what is the F1 value.

And then you can also use Shap analysis like the way I have shown to find out the relative importance of one of the specific process parameters over another in determining the predicted output. For example, here the defects we are predicting, so powder feed rate has the maximum impact more than percentage overlap, more than scan speed and power has similar impact. And then other things that we have also learned is the area under the curve. In case of training datasets, area under the curve is essentially you can see the true positive here the area under the curve is this one.

In the test case, area under the curve is this one. If it is 1.0, that means a perfect classification. If it is 0.5, that means it is one half of the area under the curve. here you can see that area under the curve is almost like 0.

86 here and this is also around the 0.88 here. this is one case for the train and one case for the test. as I said that precision, accuracy, recall and F1 value, you can see these values for both the train and test datasets, what is the value. precision is 0.867, recall is 0.963 and test dataset is perfect 1, then ROC AUC and accuracy test confusion matrix and train confusion matrix.

all those things are very clearly mentioned or very clearly summarized in this particular table and here we have used what is called logistic regression classifier,. In the logistic classifier, you are able to get this combination of precision, recall, under the curve and then accuracy test confusion matrix and train confusion matrix. Test confusion matrix is this one and train confusion matrix is essentially this one. similarly, you can essentially utilize the other classification algorithms and other classification algorithms are essentially shown here like decision tree based defect detection classification.

And this is a decision tree based defect classification. Here we have found out the overlap as a percentage overlap has much more impact compared to the powder feed rate or power or scan speed. And here again you can construct the confusion matrix for the train data and test data. And using similar kind of analysis you can essentially arrive at this particular summary table where you can see in the decision tree what is the recall value all is perfect one that means the decision tree based classifier algorithms performs much better than even earlier one the regression based classification algorithms. Another one is SVM, Support Vector Machine-Based Detection Classification.

this is in the test case it is perfect one. Train case is also it is perfect one. precision one, recall one. whenever precision recall F1 value is 1 that means ROC area under the curve that should be also 1 and accuracy also would be 1. test confusion matrix 8004 matrix, trained confusion matrix 270017 matrix. this is the summary of the logistic regression, decision tree and support vector

machine and you can certainly clearly mention that SVM actually is the best performing classifier model based on these particular parameters and then this actually predicts very well all the defect classification in this particular case.

this is the summary. summary is essentially you have the one set of input parameters, DED process parameters, you have the multitrack geometry and then we have already mentioned that what is the overlap percentage, what is the penetration area and so on. output parameters we wanted to know what is the classification models which fits best in terms of predicting that what kind of defects. that one can expect when a combination of different DED process parameters are used in real life and then we have shown that. GBM actually or SVM essentially performs much better compared to logistic regression decision tree for all these defect classifications and then SHAP interpretation is also used to find out that which parameter or which process parameter either you know scan speed, laser power, overlap percentage or powder feed rate has the most dominant impact.

compared to other parameters on the predicted output. all these analysis essentially constitute the machine learning based analysis either for regression or for classification. I hope with these two case studies, you will have now much better idea that what is the capability of machine learning models in general and how this machine learning models can be used either in predicting the melt pool geometric parameters or to predict the defects that are being generated in the weld pool in case of this multi-track weld pool either in case of stainless steel 316 or TI6Al4V or similar approach can be used for other materials for the cobalt chrome alloys or other metallic alloys which are essentially 3D printed using any of these additive manufacturing techniques. Thank you.