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

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We will continue in this lecture on the fundamentals of relevance and fundamentals of artificial intelligence machine learning in the context of additive manufacturing. what are the examples of AI/ML application? this AI/ML is expected to revolutionize our lives in general and also frontiers of the technologies in particular. if you see this automatic translation that also is given by the AI/ML, traffic prediction, web search and recommendation engines, online fraud detection, medical diagnostics very useful, text and speech recognition, image recognition, these are like in all the different examples of the real world this particularly what machine learning is expected to revolutionize. this one I have explained to you in the last lecture and I am explaining again because these are the key definitions or key aspects that you should remember. What is artificial intelligence? That science that uses algorithms and techniques leveraging computer to mimic human intelligence. Second one is machine learning like algorithms whose performance improves over time as they are exposed to more data.

That means that machine learning predictions for any AM processes where you have let us say 100 datasets are there, certain specific algorithms may work better with 100 datasets. But if you go to 1000 datasets, you will find that another algorithm perform much better in terms of the performance matrix. What is the performance matrix? I will come back to that in next few slides. therefore, the performance dynamically changes as you have more data sets in your environment or within your accessibility domain, Or whether more and more data sets you are utilizing in this machine learning predictions.

Supervised learning trained on label data, unsupervised learning it is without label, unlabeled data and then third one is reinforcement learning to take the action to change the state so that you can receive rewards. Now what is deep learning? Deep learning is a subset of machine learning where multilayer neural networks learn from a vast amount of data. deep learning is a subset of machine learning. Often many students or some of the researchers often use these terms in an interchangeable manner that is not correct. deep learning is a subset of machine learning and machine learning is again in one of the subset of large artificial intelligence that is a large umbrella.

The most important thing that I have explained in the last lecture but I am just leaving the key message here for you to remember that AI/ML is most relevant in the absence of any established relationship between dependent and independent variables. I have explained this in reference to 4D bioprinting which represents one of the most recent advances in the field of additive manufacturing. What are the key terms? What is data set? Data set is a collection of data that is used during training and testing. What is training? What is testing? I am going to explain to you soon. Hypothesis space that is set up all possible hypothesis.

Inductive learning is that inducing a general function from training examples. Evaluation that use some matrix which help analyze performance of the models. Training that are data set split used to train the model and making the system able to learn. What is training? Training is the fraction of data sets which are used to train the model. you take certain algorithm based on you are trying to develop this model and then you want the data sets to train   the   model.

that this system will be able to learn how to use this model and what is the efficacy of this model. Testing is the data set split used for evaluating the best model performance. As I mentioned in the fundamental definition of machine learning the performance becomes better and better over time when they are exposed to more number of datasets. that means if the training and testing datasets also increases or particular testing increases, the model performance also becomes better and better. K-fold cross-validation that is a resampling method that uses different portions of the training datasets and validate the model on different   iterations.

Hyperparameter tuning that is essentially choosing a set for optimum hyperparameters for a learning algorithm. training data sets and test data sets typically, Scientists have used different proportion of the training and test data sets and for various number of examples, they have found that 80-20 ratio, 80% of training data set, 20% of test data sets. I repeat, 80 to 20 ratio of training to test data sets provides optimal performance for the best model when they use the different ML algorithms. that is one message that you get. Second one, what are the inputs and outputs that I have mentioned? inputs can be either experimental data   or   modeling   data   or   computation   data   or   both.

Experimental data can be process structure property correlation shape, computational data can be generated by DFT, MD or FEA. Output, what is the output? It can be a continuous value like regression analysis can be property, the output can be printability, output can be defect. one of the major things that I am going to show you with examples from our own research that how machine learning models can be used for the defect predictions in the AM process metallic structures because lower the volume of the defects, better will be the property of the AM parts, And then this property also depends on the nature of the defects,

That I am going to explain to you in the subsequent slides where you will see that how 3D printing related experimental results and they can be better assessed by classification algorithms using that ML model. What is the historical perspective? 1764 is the birth of Bayes theorem is published. That is a probability based theory.

And this probability based theory kind of is the essentially the source of this today's artificial or the origin of today's artificial intelligence. Then comes Ada Lovelace that lays the foundation of the first algorithm. Then comes George Boole on his name that Boolean logic is being created and Boolean logic is known in today's world. Then comes Alan Turing, so this Alan Turing proposes a machine that can learn. Arthur Samuel that creates the first computer program that is IBM computer.

Madeline that first artificial neural network is created. Then Rosenberg and Sejnowski that is the neural network that is the framework. Geofrrey Hinton invents the term deep learning, around 2006 onwards. Google creates an unsupervised neural network 2012, more than 12 years ago. AlphaGO beats the first human player and then AlphaFold1 technology that is predicting protein structural scale 2018.

So you can see that every that over last several 100 years 1764 and today is 2024. over this so many years that it starts from Bayes theorem that is very fundamental theorem from there today's machine learning is essentially developed and then it is going to revolutionize human life in general. What is the basic steps of machine learning? That is some of the data like observations, measurements and training datasets. If you remember train to test datasets is 80 to 20. you have to infer some pattern or relationship within the data that is the learning pace and then make predictions regarding the previously unseen data.

consider a data set of materials for example, composition manufacturing conditions and then it has a property. And this property depending on what is the material composition, this property can be P1 to Pn. But this material composition in input, output is your property. Property you are most interested to know the property. But there are unseen things that is called fingerprint.

you generate the fingerprints while using this kind of algorithms and learn the relationship between composition and manufacturing density and predict the density of property of new untested materials with arbitrary compositions on manufacturing. as I said that machine learning is a branch of artificial intelligence that is concerned with the design and development of algorithms that allow computers to evolve behavior based on empirical data. One of the things that you learnt in the previous slides is that performance improves over time more data. in the traditional programming let us say C or C++ programming what would happen that you keep the data and you give the program then you get an output

right that computer will run the code that program and then you get the output. In the machine learning, what you have learnt already, the training is 80% data.

You split the datasets into training and testing. With the training data, you allow the system to learn from these datasets. Then you generate learning methods and then testing data is feed into this. Then it is able to predict. you get the data, you get the output of this one learning   method.

Then you essentially generate a program here using computer.   without even programming, you can run this particularly develop this machine learning model that is what has been also mentioned to you earlier. basic workflow in the machine learning model, this is like a generic description. you have a raw data. in the raw data, you have to see the dimensionality reduction or extraction features and output, then you have to split the   raw   data,   training,   test   data.

You can also keep some amount of data, percentage of data as validating sets. training data essentially train the model and this particular model there are different model like hyperparameter selection and validation. I will show you more examples of that. And test data that 20% data that is what has been mentioned that is allows you to estimate this model. And then there is a new instances and then final model and predicted output.

 first phase is your extraction phase, second phase is your training phase, third phase is your prediction phase. But the question is reliability of the prediction. how reliable is your predictions. You can predict many things but whether these predictions is statistically reliable, what are the performance metrics that you consider which allows you to be also convinced about the machine learning based predictions and what you have to believe and you have to trust the data,   therefore, input data quality is very important   otherwise as you know in that conventional programming what we learnt in the undergraduate student garbage in, garbage out. if your garbage is into the program the output also will be the garbage   right.

 therefore one has to be very very clear about the quality of the input data. what data you are taking and whether you are randomly choosing without any bias, 80 percent the training data sets and 20 percent the testing, the moment that you actually allow your personal bias to be involved in the dataset creation, testing and training datasets that actually bound to give you these unrealistic predictions or unreliable predictions. That is the better word, unreliable predictions. performance matrix, over the time that you have learnt in this last lectures, this todays lecture, that performance of the machine learning becomes better and better over time as it is exposed to more and more amount of data. Then question is that how you can define performance matrix or how you can evaluate the performance of any

machine   learning   model   per   se.

one is that R square. Now, R square is the term that you have learnt in your basic course on statistics, correlation, or here you can also see coefficient of determination, Coefficient of determination or sum of the squares of residuals divided by total sum of squares and then you have to deduct from 1 unit, so then you get R square. R square should be close to 1 so that means it should be close to 0.95 to 0.99 or somewhere like that.

That is the best performing model. Then second performance so here you can see that this is that ideal line 45 degree line if you plot actual versus predicted. data is scattered across this 45 degree line and then if you get actual versus predicted this data is scattered and therefore you can see that this how you can establish the statistically reliable performance parameters, performance matrix and this one of them is R square. Second one is the root mean square error RMSE. RMSE it is 1 by n, sigma i is equal to 1 to n, yi minus yi average hat square and that is 1 by n is this, you have to divide it by 1 by n. So this particular formula   it   is   called   root   mean   square   error.

This value should be close to 0.0. if it is close to 0, R square is close to 1 that is the best performing model. The third one is that the residual error distribution. what you see here from actual to predicted here I refer to this particular plot again. your actual data points is somewhere here and the predicted data points is there. this minus this will give you error for   all   these   different   data   points.

what is the residual error and what is the probability density of this residual error and as long as this residual error distribution gives you a good Gaussian type of distribution that is more like uniform Gaussian type of distribution that means that particular model will give you best predictable results. I repeat three parameters one is R square One is RMSE, third one is the residual error that has been just explained that it should be Gaussian distribution. And here you can see two different type of columns are there which are being plotted and these columns have different color and one is for the testing datasets and one is for the training datasets. training is this one, the larger column and testing is this one. Both for testing and training it should give rise ideally to Gaussian distributions and then you can consider that this particular machine learning model that you have generated that will   likely   to   give   you   the   reliable   predictions.

this is that residuals calculated for training and testing data sets, good residual plot, high density of points close to origin and symmetric about origin. And best performance as I mentioned close to 1, RMSE close to 0. And this is the residual error distribution. You see that it should be close to 0, so that maximum density. if you take the probability density This is the highest probability density you can see close to 0 right and this is the residual

error   distributions.

Epsilon is the residual error and X is that essentially measurement that actually what I said that actual versus predicted. This is the actual, this is the predicted. in the predicted distributions in the predicted data what is the residual error distribution if the maximum is close to 0 origin and then symmetric about origin or origin means 0, 0 and this is also 0, 0 then it is a best performing ML model. this is the criteria for the best performing ML model Now, training and testing dataset, generic rule is that training is the process of making the system able to learn. there is no free lunch rule that is applicable to training.

Training set and testing set come from the same distribution based on specific assumptions or bias. I mentioned to you before that there should not be any human biases involved when you randomly distribute 80% training dataset, 20% testing dataset. The moment you apply your bias, you are bound to get unreliable predictions. Performance, there are several factors like types of training provided, background knowledge, type of feedback and learning algorithms used. Two important factors here, one is the modeling and one is optimization.

suppose this is a universal data sets, this is the overall data sets and you get the data acquisition then you distribute it. training datasets and testing datasets are essentially unobserved datasets. Then you essentially distribute 20% of testing datasets. Algorithms, I mentioned before that it can be supervised learning that is prediction and classification. classification is essentially discrete levels and regression is the real values.

there are two major things in the supervised learning. Classification algorithms, example is the defect predictions in the AM parts additive manufactured parts. Regression classic example is that you vary the process parameters you would be able to see that what is the weld pool depth, weld pool height, weld pool area and so on and so forth. Unsupervised learning, this is the concept of supervised learning. Unsupervised learning, I am talking about   this   now.

Unsupervised learning is the clustering. it is a small domain clustering, probability distribution estimation, dimension reduction and so on. Semi-supervised learning or reinforcement learning is the decision making and also for class machine. Supervised learning overview, the supervised learning model mapping from one or more inputs to one or more outputs and model is a family of equations. Computing the inputs from outputs that   you   give   inferences.

Model also includes parameters. Parameters affect output of the equations, And training a model is essentially finding a parameters that predict outputs well. This well word

essentially is very important and it is not a qualitative term. It should be statistically reliable and also it is good predictability. Good means it is trustworthy predictability. x is actually a input, y is output, the model is equal to $y = f[x]$.

x is essentially functional square brackets that is how it is to be learned, normal is returns vector, bold is returns vector, capital bold is returns matrix, any times if you put capital X that means it is a matrix. training data set from i pairs of input-output variable, so this has been shown here, let us say x_i, y_i, then ii is equal to 1, loss functions or cost function measures, now bad model that is also has been shown here on short, in short, for short it is L phi that returns a scalar that is smaller when model maps inputs to outputs better. it decreases this value decreases when the model performs better and better that is the major message that I am going to tell you. Regression, this in traditional sense regression essentially means model input connected to model output through a model and or real world output. this is the example, it is a laser power, scan speed, layer thickness, hatch spacing that is for example in the metal additive manufacturing, Let us say SLM.

it gives you 4 values like different values, then it gives you 340 like a data sets, then you get the geometry, melt pool, density, porosity, roughness, mechanical properties, yield strength, ultimate tensile strength or percentage elongation to failure. there is a univariate regression model like one output real value and multivariate regression model that is multiple outputs and real value. this is the question for regression analysis which I am going to show you with real experimental results particularly with case of supervised learning models later on. Now examples of the 1D linear regression model, for example it is a simple linear model y is equal to phi 0 plus phi 1x, so where is x is the input variable, phi functions is phi 0 phi 1, so this is y offset and that is the slope of this one. Examples of the 1D linear regression testing, this is the output, this is the input x, y versus x and then you see that there is a variation there.

degree to which this is the same as training that is called generalization and often it should not lead to overfitting or underfitting. It should be just fitting the data with this particular model examples. K-fold cross-validation, these are like more advanced topics in the machine learning. as I said that you know there should not be any bias and particularly training datasets and testing datasets that we need to take care of the overlapping of the test datasets. what is the first step? You split the data into K subsets of equal size.

And this k-fold cross-validation means this is essentially k subsets of equal size of the data. Second step is that use each subsets in turn for testing the remainder of training. This means learning algorithm is applied to k different training sets. here for example in the training sets if you see this is the MSE1.

this is the mean of this particular training data sets. this is the training fault, this is the validation faults. you randomly put this MSE1 to MSE5 like that you know that k different models. Then you essentially use the best model and while selecting the best model, then you use the different ML models like KNN. K nearest neighbors, SvM support vector machine, ANN artificial neural network, DT decision tree, RF is the random forest model, GBM is a gradient boosting machine and you learn later on there is something called tree based model.

learning models which is a more generic term. you put these best models, your training datasets you apply, you try to fit it, then you develop the capability to predict the some of the test dataset that prediction goes to the final models. often the substrates are stratified before cross-validation is performed to yield stratified k-fold cross-validation. And then error estimates are averaged to yield an overall error estimate because error estimation that I have mentioned to you with this error distribution that distribution of the residual error that is important and residual error distribution should be Gaussian in nature. with the maximum probability close to origin 0,0 and also this should have a Gaussian type of distribution both for training datasets and testing datasets.

One of the classic example is linear regression. Even when people did not know about this machine learning, artificial intelligence, linear regression has been used in statistics for quite long, for many decades or centuries I would say. linear regression as the name suggests, you know y is equal to mx plus c that is classic equation for describing a line. m is the slope, x is the y-intercept and y is equal to mx plus c. here what you can see here it is y is equal to a0 is your line intercept, a1 is the slope linear and a1 is linear regression coefficient and epsilon is your random error while predicting the target variable y and x is your independent variable. mean squared error essentially what you have seen here this is the mean squared error MSE is essentially mean squared error when I have mentioned while describing this k fold cross validation in the last slide.

mean squared error is nothing but 1 by n is sigma i is equal to 1 to n yi minus ai xi plus a0 square. And that means that, you know, you put yi here, this minus a0 is this essentially the residual error square, this mean square error. And n is that size of your datasets. gradient descent that is used to minimize the mean square error by calculating the gradient of the cost function. this is your cost function and then use gradient descends to update linear coefficients by reducing cost function.

This is some examples that slope is phi1 and intercept is phi0, so how this loss function will evolve that is L phi. You remember this L phi in some of the earlier things that I have mentioned that L phi is the loss function and it decreases typically as the model performs better and better . this is the performance matrix that I have already mentioned. Another

thing that has been mentioned here, for example, just I am giving you different example, here loss capital L is the value of 0.

19, here phi 0. what is phi 0 and phi 1? Phi 0 and phi 1, I think I have defined you before phi 0 and phi 1 essentially are you can consider this like A0 and A1 here. this is the essentially output data, this directly plotted in a borderline, these are like scattered data points. this dotted line essentially indicates what is the deviation from the predicted with the real one. this is least squares loss function. L phi is a function of xi phi minus yi that square and this for the large number data sets i is equal to 1 to y it is phi naught plus phi 1 xi minus yi square.

essentially it gives rise to something called epsilon that is a residual error right that is square. 1D regression function again it shows a different way of representing the same thing here along this is a 3D plot L5 versus slope phi1 versus intercept phi0 that is also just to show or illustrate the example of 1D linear regression loss function. I stop here. I will continue in the next class again with some of the remaining concepts with examples of the artificial intelligence and machine learning. Thank you.