Particle Characterization

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Module No. # 02
Lecture No. # 05
Morphological Characterization: Decision rules

Good morning and welcome to the fifth lecture in our particle characterization course. In the last two lectures, we have been talking about shape characterization, and in the last lecture, we reviewed several classes of methods to characterize particle shape as well as several subcategories within these classes of methods, ranging all the way from very sophisticated mathematical techniques to very simple characterization of bulk properties of powders, rather than the properties of the individual particles.

In this lecture, we are going to focus on how a systematic approach can be applied to the characterization of particle shape. Now, when you think about shape characterization, what it is, it is really an exercise in pattern recognition. A particle has a certain pattern around its outer surface, which is what we call it shape. So, there are many methods that have been developed for pattern recognition, in general, and many of these methods are also applicable to shape characterization.

So, we will describe some of these methods today. Now, when you talk of pattern recognition, in general, not even a supply to shape characterization, but pattern recognition in general, how do you do pattern recognition? While there are really two key aspects to it - one is that you should have a choice, a selection of pattern that you can match the pattern that you are interested in to and make certain evaluations regarding how well the pattern that you are examining fits one of these candidates patterns.

So, the first requirement is the availability of candidate patterns to compare to, and the second is the formation of certain decision rules or criteria, which will then, which you can then apply to decide how well the test pattern fits one of these candidates pattern, right? So, the two key aspects are having a selection of candidate patterns and then the formation of a decision rules or criteria that will enable us to decide how well all patterns fits one of these available patterns.

So, when we, when we think about pattern recognition in that sense, obviously shape characterization fits in very well, because again shape is just a pattern really; it is the pattern that the outer surface of the object fits. So, we should be able to take these general guidelines for pattern recognition and apply them to shape characterization as well. So, how do we do that? I mean, suppose you are trying to do pattern recognition as a way to determine particle shape, what are the key elements in this approach? Well the first is the definition or identification of candidate particle shapes. So, you should have a library of shapes that you can choose from.

So, that is essentially the first element and I think a lot of work has been done in this area of shape characterization that – yes, we do have a library of thousands of shapes that we can compare to. The second is the formation of the decision rules or criteria. What kind of quantitative measures can you adapt to decide whether the shape that you are looking at is close enough to one of these candidate shapes?

And that is the aspects that we will actually focus on the most in this lecture, because there are again several classes of these decision rules or criteria that we can apply for shape characterization, but let say that you already have these two. You have a set of shapes to compare to and you have certain criteria or decision rules that you can apply. The, what is the next element in our in our approach?

The next element is for an observer to collect data. You have to collect data you have to collect data on the shape of the particle from which you can then extract the valuable information that you need. Now, when you collect data, in general, not just for shape characterization but for any purpose, not all the data that you collect is ultimately going to be relevant. You will collect data that are relevant; you will also collect a lot of data that are not. So, the second job that the observer has to do after collecting and recording the data - the observer has to sort the data, and essentially, distinguish relevant data from irrelevant data.

So, you only take the data there is relevant for shape characterization and then you start applying your decision rules to the set of relevant data and the way you do it is very similar to how we would numerically solve a differential equation. For example, you look for convergence, so, you start with an initial guess at the shape of the particle and then you compare it to various, well the data that you have obtained

And see if you are, if the, if the data that you have taken, the relevant data that you have taken matches the profile that you have selected. If not, you iterate. So, you either change the, comparison, comparison shapes slightly to see the fit improves or you collect data, more data. So, by essentially doing more experimental observations as well as by considering more candidates shapes, you go through an iterative process until you converge to what is the actual shape of the particle that we are looking at.

So, very broadly these are the key elements of a pattern recognition approach to particle shape characterization. Now, if you want to take this approach and caste it in the form a systematic procedure, what are the key steps in such a procedure? The first step is really what we call? A gross examination of the particle.

So, this can be done by an untrained operator. This can be done without any resort to high level magnifications or sophisticated lighting and all that. So, it is a matter of a simple close visual examination, and for a surprisingly large percentage of times, that is adequate. So, you know somebody who is skilled but not necessarily formally trained, somebody who is experienced can actually do a simple visual inspection of an object and quickly determine its shape, because as I mentioned earlier lectures, the human eye is the most sensitive shape detection instrument.

And so at that stage, you take a step back and ask yourself is that sufficient. Somebody with a trained eye has looked at this object and made a suggestion regarding its shape, is that sufficient for my purpose or do I now want to go deeper and collect more data and do more investigation.

So, the answer is no, then you are done. You record the shape and you are done with it. If he say yes, then again you go into this step by step scheme on forming your decision rules, identifying a set of objects to compare to and repeating the comparison process in an iterative way till you converge to a shape that you are happy with it.

So, these are the various steps, in a, in a systematic process for doing shape assessment. So, as I was mentioning, the key in all these is the decision rules or criteria that you use to decide when you have converged to the actual shape of the object. Now, it turns out there are broadly eight methods of doing this. So, will list those and then we will come back and discuss those in more detail.

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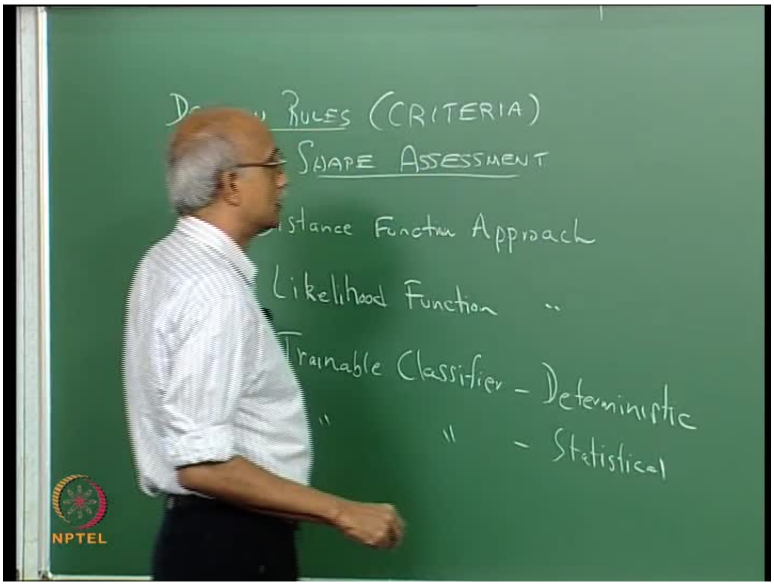

The first method is known as Distance Function Approach. The second method is known as Likelihood Function Approach. The third is Trainable Classifier Deterministic. Fourth is Trainable Classifier Statistical.

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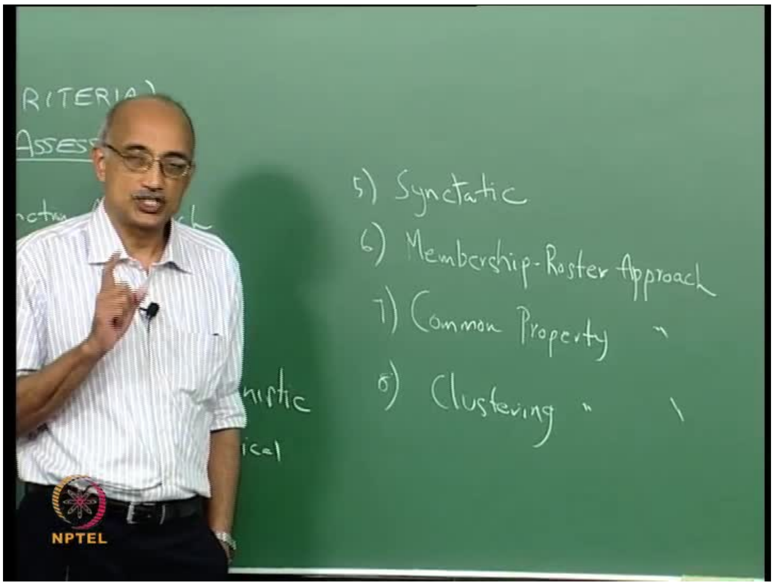

The fifth is Synctatic Approach. Sixth is Membership-Roster Approach and the seventh is Common Property Approach and the last one is Clustering Property Approach.

So, these 8 actually represent, in, in a very broad sense, all the methods that are used to provide comparisons of the actual shape of your object to several available shapes in a library so that you can decide which shape most closely approximates the shape of the particle that you are actually analyzing.

So, let us take these in order and look at how they work. So, first one distance function. The way you want to think about it is that, it is, it is very similar in concept to, for example, any pattern recognition analysis.

The first thing you have to decide is what is the appropriate space that you want to look at? It is not the dimensional space. What you want to look at here is a space that as coordinates that represent certain shape characteristics.

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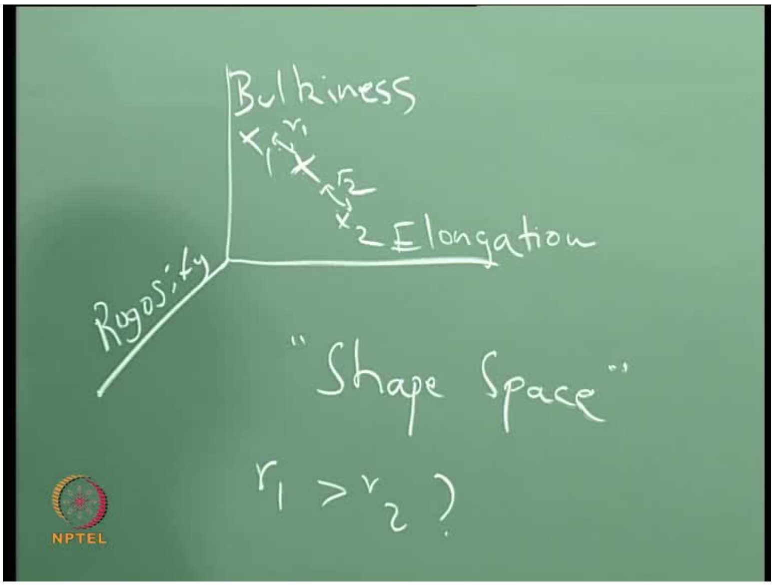

For example, you could take a three-dimensional space, in which, let us say one axis is Elongation; the second axis is let us say the surface roughness or Rugosity and let us say the third one is Bulkiness. Now, something like this is called a Shape Space. It is just like physical space except that X Y and Z coordinates have been replaced by certain shape parameters.

So now, what do you do in this case? Well you take the object whose shape you are trying to assess and find its location in this space. In other words, it will have a certain bulkiness characteristic; it will have a certain elongation characteristic and it will have a certain rugosity characteristic.

So, let us say that the shape that you want to assess is some x and it is located at some point in this three-dimensional space. Then, again from your library or from your experience, you select two shapes that you think most closely approximate this shape, because remember that each shape is unique.

So, this particular point in this three-dimensional space will not be available in your library, you know, unless you get extremely lucky and unless your data is inaccurate, because it is physically impossible to have two particles that have the same shape, right?

So, there always be a deviation, but what you do is you select one shape. Let us say it is somewhere here and a second shape that somewhere here. Now, how do you choose these coordinates? Why did we pick these three particular shape parameters? Remember, the sorting by relevance, you have to, when you characterize shape, it is, you know, in a way it is like the blind man and the elephant, right? I mean you can define shape in so many ways. So, you have to pick the shape characteristics that are most relevant to the physical problem at hand and also try to reduce the number of dimensions as much as possible. For example, if only two of these shape parameters are really relevant for your process or your problem, then just do a 2D analysis, do not even try for a 3D analysis.

But certainly if you go beyond 3 D, I think you are going to complicate your problem quite a bit and its very unlikely that any physical process or problem will involve more than three shape parameters as relevant parameters. It is very important that you have to be able to decide what are relevant and what are not relevant for the problem at hand. So, in this particular case, we have decided that these three parameters are very critical to the problem we are trying to solve and that is why we came up with this particular shape space.

So, what is the next step? You essentially find the distance, let say r1 between X1 and X1 and r2 between X and X2 and you compare them r1 greater than r2 or r1 less than r2, whichever is smaller your shape is obviously closer to that candidate shape. So, you discard, let say that r1 is greater than r2. So, you will discard X1. Now, you choose a third shape X3 which is let say closer to X2 in a way, right?

And now you take r3 when you compare r3 and r2 and again see which one is larger and let us say that now again r3 is larger; so, again you discard this, and so, you know basically retry to process still you find a particular shape that gives you the minimum in this distance. So, this is what is known as a distance function approach to obtaining the shape. You keep identifying the target shapes, identifying the so called distance in the shape space between the candidate object shape and the real shape at hand, and then, you use essential a minimization algorithm to minimize this value of R the distance between the actual object and the comparison objects. Now, what is the second method?

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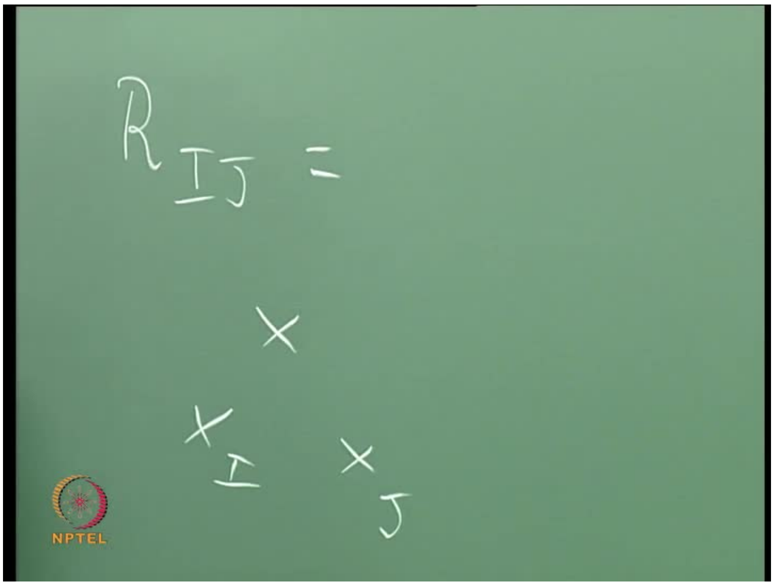

The likelihood function method - it is actually not to dissimilar from this approach but with one key difference. This is what we would call deterministic approach. You figure that you know exactly what your X value is and you know exactly what X1 is and you know what exactly X2 is, and so, everything is deterministic in nature.

You are not allowing for uncertainties in your data but real life does not work like that. So, most of the time what you deal with are probabilities. So, instead of trying to minimize this distance, another approach would be to say you look at the probability of the shape of your particle fitting one of the candidate shapes and what is the error associated with assuming that the shape of your object corresponds to particular reference shape and you try to evaluate this error for various shapes, and then, you try to minimize the error involved in your selection.

So, the Likelihood Function basically evaluates a loss parameter R I J, which is really has two components - the first is supposing you have a shape i and you have a shape x and you are trying to compare it to some X I and X J shapes, right? And let say that you assign x 2 x i. Now, the error involved in that or the loss function is if it actually belongs to shape x j but you have miss classified it as belonging to x i, right?

So, that is one type of error. The other type of error of course is if x actually belongs to x i but you have misclassified it as belonging to some other shape category. So, there are really two types of misclassification errors that are possible in general, but in this particular case, will just take into account the error where l really belongs or the x really belongs to x i but you have taken it to belong to x j and we represent that by l i j parameter and that is also a probability of x belonging to x i.

So, the higher the probability that you assign to x belonging to x I and the higher the error associated with misclassification; the higher will be the overall loss parameter, right? So, this is the last function associated with misclassification between two shapes. Now, similarly, for all the various candidate shapes, you can define these R I J values. So, for a particular I value, for various J values, you can calculate these errors, and ultimately, the way this works is you try to minimize the net error that you make due to misclassification.

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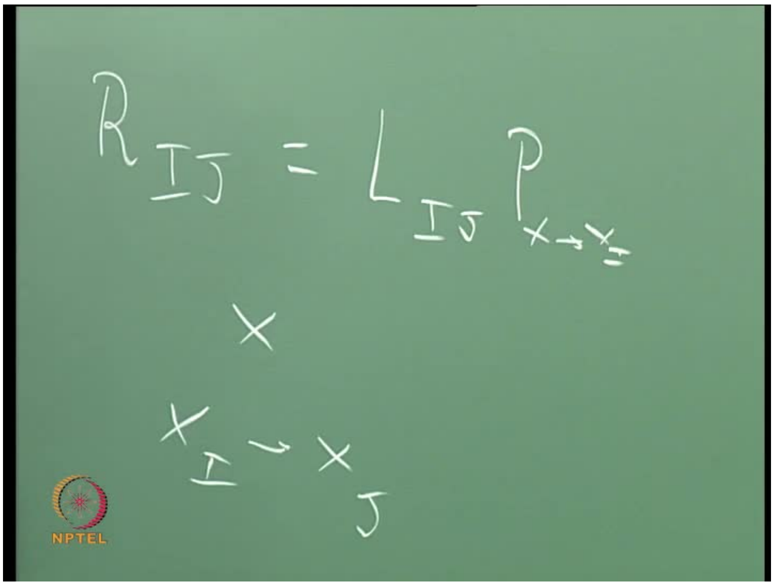

So, it is a probability-based approach which takes into account again two things: the probability, that the shape of the object or the shape of the particle belongs to a particular reference shape; the error that you make, when you make that assumption, and the error associated in misclassification of wrongly classifying it to belong to a particular shape.

And so, you look at the error associated with misclassifying a particle of a particular shape into all the other shapes that are present and that is why the summation comes in and you eliminate and you estimate the total error and you do this for by comparing x to all each of the particle shapes that are available. So, whichever classification results in minimum error is the one that we take to be the ultimate shape of the particle.

So, that is the way a statistical classifier or a likelihood classifier works. It is trying to maximize the likelihood that your choice is correct. It is not saying that it is absolutely correct, because whole point behind the statistical approach is that you do not know in an absolute sense, you know nothing is hundred percent guarantee, but what you can do at this type of analysis is to say that my certainty that it belongs to this particular shape group is greater than my certainty that it belongs to any other shape group, right? That is basically the only conclusion or declaration you can make at the end of such an exercise. Ok.

The third and fourth methods are trainable methods. Now, what do we mean by that? I think if you have dealt with for example neural networks in solving problems, it is essentially a learning algorithm. So, you start with, in the, in the case of trainable classifier, in the case of the trainable classifier deterministic method, the way you would do this is again you will take to initial guesses for the shape of the particle.

And you will compare them to the actual shape at hand and you will estimate the delta between them, the differential between yours chosen shape and the actually shape and you will look at which of these two initial guesses is far that is. So, in that sense, it is similar to a likelihood function.

The difference though is that instead of you going an arbitrarily selecting a third shape, the algorithm is setup in a such a way that it automatically looks at the difference between the actual shape and the two initial guesses disgorge one of the guesses and iterates the other guess to provide a better fit to the actual shape at hand.

So, it is going to learning as it goes along. It looks at how bad the initial guess was or how far the initial guess was from the reality and it does the adjustment on the flight so that you converge to the real shape as quickly as possible. So, instead of just dumbly or arbitrarily choosing various shapes of comparison, you set it up as a as a learning algorithm which will try to converge to the actual shape as rapidly as possible.

And the trainable classifier statistical again is the equivalent to our Likelihood Function method. So, here again instead of choosing shapes arbitrarily and looking at the probabilities associated with either classifying or misclassifying, you allow the algorithm to choose these shapes in a progressive way by looking at the statistics and trying to minimize the probability of making an error.

So, these two cases are trainable or learning types of algorithms which in principle should enable you to converge to the real shape much faster compare to the first two methods which are classical or traditional methods, where the observer or the analyst makes a choice of candidate shapes and so on.

Now, as people that have used this type of approach in solving other type of problems, if you have ever done it, you know this method these methods are not full proof. Can you trust a mathematical algorithm to learn and converge faster to the solution? I do not know. That is actually questionable. There are cases where this approach can actually lead to a slower approach to convergence than one where essentially as a user you are making the guesses, because when an algorithm like this tries to learn, depending on the complexity of the problem, depending on the conflux within the problem, you can very easily diverge rather than converge to the to the real solution.

But there are certainly many situations where these so called the trainable methods have found why it is produced. The fifth method Synctatic again goes back to verbal descriptions, but with one change. Instead of simply looking at the shape of the particle and calling it, you know a disk or a rod or a cylinder or a ellipsoid or whatever, you try to base your decision on the origin of the particle.

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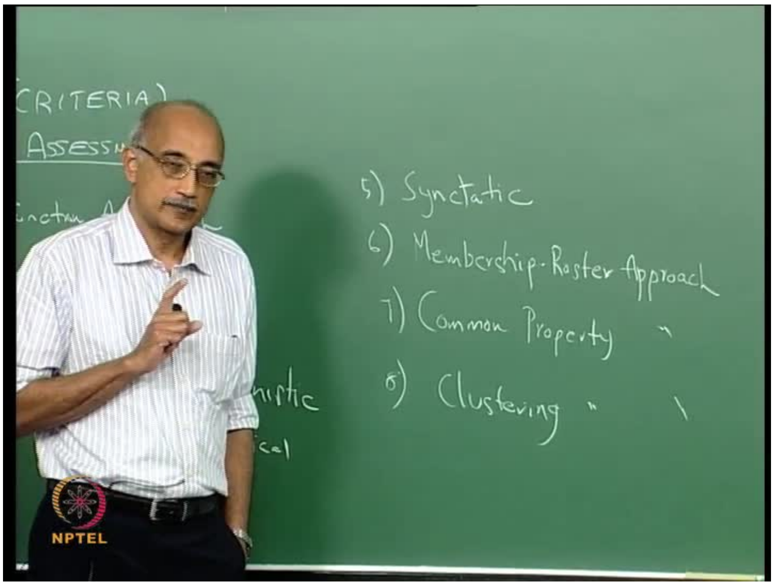

For example, if you know that the process which generated this particle involved condensation from a vapour, right? Then, you can actually use your physical insight into that process to arrive at a shape estimate for the object. If you look at surface energy minimization of when you, when you are condensing a droplet or a solid particle from the vapour phase, the most likely shape is spherical in nature. So, your first guess for the shape would be spherical and then you would, you would compare the particle shape to it, and if it is close enough, you will just call it a sphere like or spherical and move on.

If you do not need to be very quantitative about it, you know if you do not need a quantitative index for sphericity, then this type of decision regarding the shape based on your physical insight and being able to provide the description in a verbal or descriptive manner is sufficient and actually far superior to other methods, because the advantage of this approach is you are actually using your physical insight into what is happening to decide the shape rather than doing it completely arbitrarily. In other words, shape assessment in this case moves from that domain of mathematicians to the domain of the scientist who knows something about the process that is going on.

Another example is - if a you are generating the particles by a grinding process, then the most likely shaped is going to be crystalline, because the fracture is going to happen along certain lines or gradients that are present in your, in your material. So, the most likely shaped is going to be elongated or crystalline, in, in nature. So, the Synctatic methods combine verbal descriptions with physical inside to quickly formulate your initial guesses for the shape of the particle.

Now, what do we mean by the membership roster approach? So, number 6 - membership roster. Well it is based on a very interesting concept. Now, when you look at clubs, let say you become a member. Now, in a traditional way, you would say that you can either be a member or a non-member, right? So, you have a club and if you belong to the club, you are a member. If you do not, you are a non-member. So, if you if you define a membership index, it is very binary, right? It is either 0 or 1.

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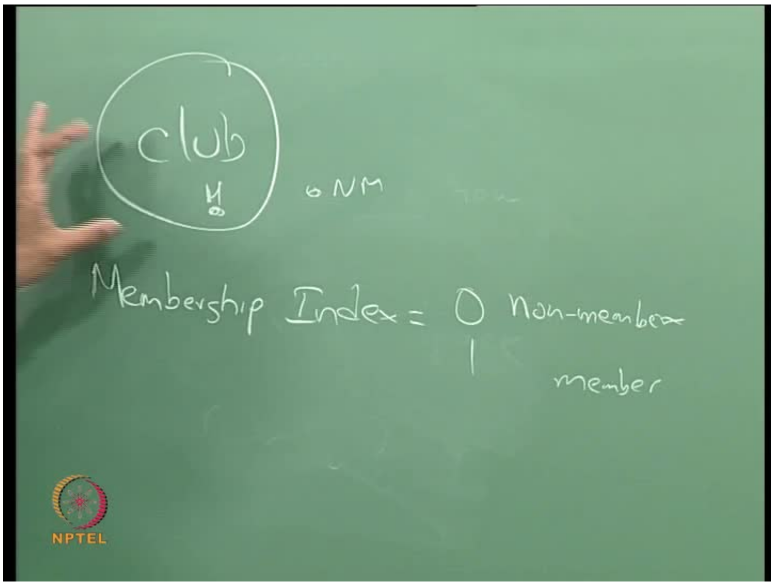

It is 0 for a non-member and it is equals to 1 if you are a member. Now, what relevance this is have for shape assessment? Let say that this is the reference shape and this is the shape that you are analyzing. You can either say that the shape you are analyzing belongs to that reference shape class or it does not, right? That is a very deterministic way once again of looking at shape characterization. It is either belonging to a shape or it is not. Now, the problem with that is that shape is not a binary phenomenon, you know, there are essentially infinite shades of shape.

So, this type of a binary approach is actually not appropriate for shape characterization. Now, again going back to club and being members, you can also talk about various grades of member ship, right?

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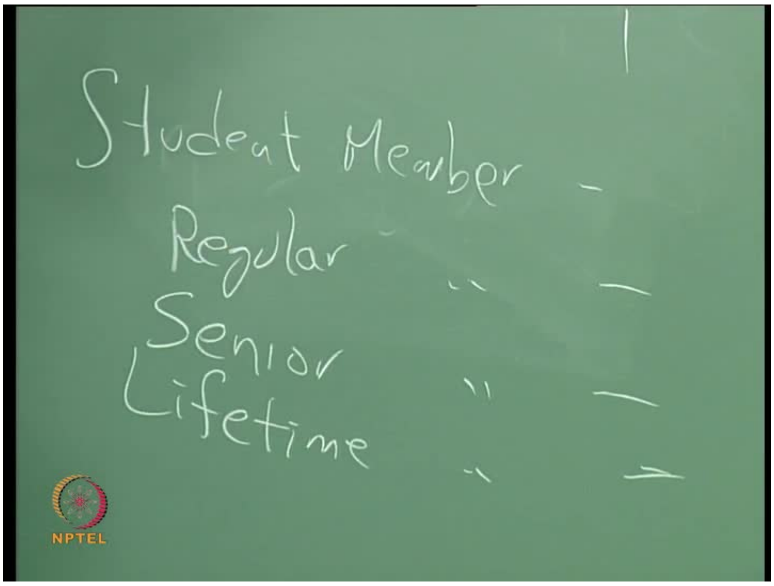

So, for example, in a club let us say you are a Student Member; which means that you get certain privileges but not all, and then, you are a Regular Member; then you are, let us say a Senior Member and let us say you are a Life Time Member and let us say that your member ship privileges depend on the class of member ship that you have.

So, here, you do not just go from 0 to 1, instead – yeah, if you are a non-member, let say that, that is a zero, but let say that you can become a student member which will give you certain rights and privileges but not all of them.

So, the index here may be a 0.2, and let say that as a regular member you get virtually all the benefits but may be not all of them. So, this may be a member ship index of 0.7, and let say there as a senior member, you get 90 percent of the benefits, but you really have to be a life time member or a founder member to get all the benefits, right?

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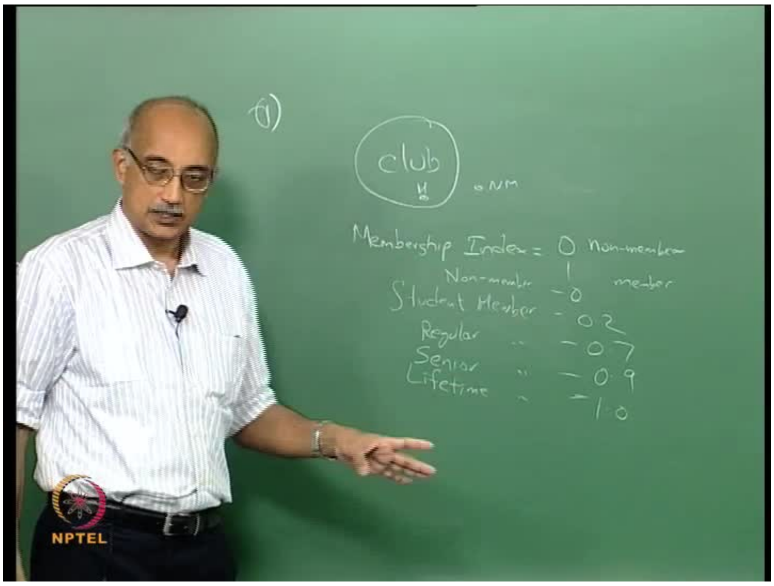

So, here what we have done is change this from a binary system of member ship to essentially continuum of membership and this type of membership concept is known as fuzzy membership and I am sure you have studied set theory and you know about fuzzy sets, right? It is something very similar in concept. Now, the advantage of this approach is it enables us to compare a reference shape to the test shape, and we do not have to say 0 or 1, we can actually say this shape corresponds 60 percent to the shape that i am looking in.

So, you can actually assign it a member ship index which is not 0 or 1 but somewhere between the 2. So, let us say again that you have multiple shapes that you are comparing to and you compute this member ship index for each of these candidates shapes, and let us say that the member ship index here is 0.7; here it is 0.8; here it is 0.9 and so on, right?

So, once you have done this exercise, what you conclude? The shape is more likely to belong to the one which has the highest membership index, but you do not have to stop there, because then what you do - take the two shapes that have the highest membership indices and look at the cross section of these shapes, because the concept here is if this shape as a lot in commonality with this and a lot of commonality with this, then if you just define a new set, that combines a common elements of these two; then the likelihood of this belonging to that new set that you have a generated is going to be even higher.

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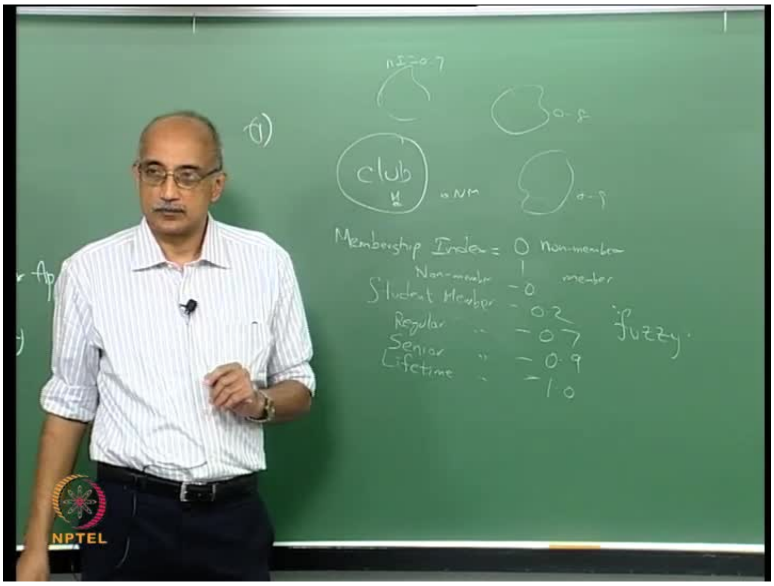

So, if I take, a, the cross section of these two, and you will compute the membership index, it is likely to be greater than 0.9 or 0.8. So, it may be as much as 0.9 let say, and again this can be done iteratively depends on where you want to stop. If you are happy with 99 percent convergent, you can stop right there, or if you want better, then you compare the new set that you have generated and one of the earlier sets and again look for cross sections between these shapes and you keep repeating this until you get as close to one as you want, right? So, this, this fuzzy member ship concept is very successfully applied to particle shape characterization, because by its nature, particle shape is a fuzzy characteristic, ok?

Now, the seventh approach what we call that common property approach. Basically what it implies is that if you are comparing the shape of a particle to various reference shapes, the reference shape that is likely to be closest to the shape of the particle you are analyzing, is the one that will have the maximum number of common properties.

So, what do we mean by that? Well let us say that you have a particle that has a certain, you know, again, let us it is say certain bulkiness, certain sphericity, certain roughness, and let say that these you have decided are the most relevant characteristics of the particle from a shape view point.

And you look at n different objects, and instead of computing a distance from the object in in a space and so on, look for actual commonality. See the problem with the distance function approach is that it is somewhat empirical in nature. In other words, you can have a situation where you are comparing a particle into two shapes visually. The particle may actually be very close to one of the shapes, but when you actually go through once these quantitative analysis, the conclusion you come to may be completely different. You may actually choose the other shape based on quantitative computations, because you can, the two do not have to match exactly, because all you are trying to do is minimize the total difference between the objects. Whereas, this approach basically says you give more weightage to absolute coincidence of one or more properties of the reference shape.

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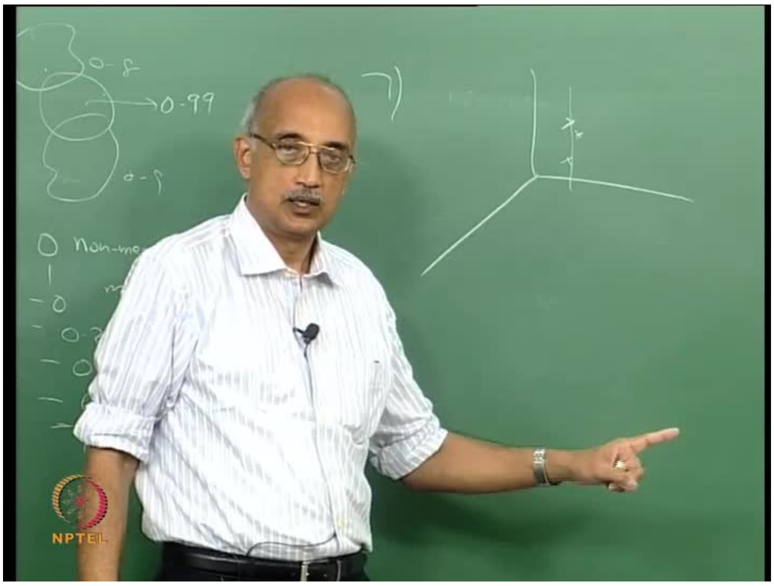

So, what do we mean by that? So, in this approach number seven, again you go back to that 3D space with three shape characteristics forming the coordinates, and let us say that X happens to be here, right? Now, when we do either the distance formulae distance function approach or any of these earlier approaches, that the shape that you finally decide naturally we somewhere here, and the reason being that, that is the point which actually gives you the minimum deviation in the three-dimensional sense from the object that you are analyzing.

However, the problem is this does not correspond to this in any of the three parameters, right? The X is different; Y is different and Z is different.

So, if you are just doing visual inspection, another particle which may be further in terms of distance but exactly align with it on at least one of the axis just visually you will probably conclude that is a better, right? Because you are not mentally doing all the mathematics, you are just intuitively observing and deciding, and it happens that for this candidate at least one of the three parameters is aligned exactly with the object that you are trying to analyze, and so, the common property approach basically says give more weightage to exact alignment of at least one of the relevant properties of your reference shape to the corresponding property of the particle that you are analyzing.

So, do you understand the difference between two approaches? This approach is purely mathematical in nature. It does not give any weightage to you know the human intuition or human observation, mean for example, if this access is sphericity, you would decide that a reference shape that has the same sphericity as this is the one that may catch your eye more than anything else and that may be again the most relevant, and so, you would have probably pick this as the actual shape and not this even though from a three-dimensional distance or likelihood view point, this is mathematically a much better fit to the particle that you are trying to analyze.

So, the key difference again is the common property approach says do not worry too much about mathematically minimizing the deviation of the reference object from your object, but instead, the even more decisive on what are the critical shape characteristics for your process and try to home in on a shape that gives you one exact match in terms of this characteristics.

Even though that the net deviation may be greater. The last approach, the clustering approach is again very similar to the common property approach in the sense that it says even more clearly what you look for is a clustering of particle of characteristics. That is very similar between your test object and reference object. So, here again, if you look at this shape space type of analysis, you take your object that you are trying to analyze and let us say that you evaluate its properties and it comes to a particular location. Now, let us say you choose ten different reference objects and you find that they all lead to various property or locations that may be in different places in this space, right?

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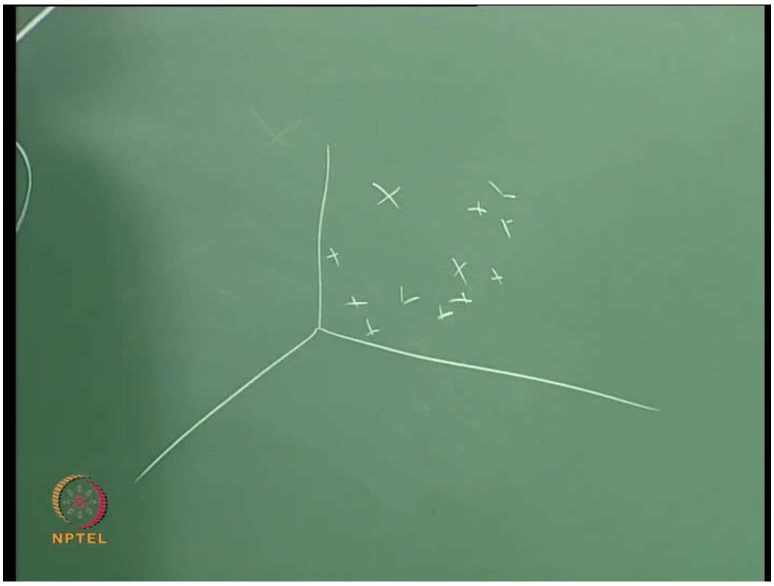

So, this is your object that whose shape you are trying to analyze and these are the candidate objects. Now, what the clustering approach says is that the shapes that you are comparing to should be clustered in the shape space. In an area, there is adjacent to the particle whose shape you are trying to analyze.

So, of these shapes the once that I would essentially short list so to speak are those that show clustering in the shape space, that is, as adjacent to the test particle as possible. So, in this particular case, I would probably choose certain objects that show very similar clustering of properties compare to the particle that I am trying to analyze.

Now, what is the difference between your common property analysis and clustering analysis? In common property analysis, again the point is you are trying to minimize the number of properties that you want to exactly simulate. So, that works well when there is one predominant shape characteristic that is most relevant. So, because then you can essentially choose a reference object that has virtually an absolute agreement with your test particle for that particular aspect.

The clustering approach works when you have more than one property that is relevant, and but at the same time, you do not want to do this on a purely empirical mathematical manner. You still want to carry over certain aspects of the common property approach, but in this case, you identify the minimum number of relevant shape characteristics. Find out of all the shapes that you are considering which one is have the closest clustering of these properties to the particle that you are trying to analysis.

So, both these approaches differ from the first two approaches of distance function and likelihood function and so on in the sense that they give more weightage to the physical or visual appearance of the particle rather than a purely mathematically based minimization algorithm. I mentioned yesterday that, for example, when you digitize a particle profile and you do a polynomial fit, the shape that you come up with may be completely different from the actual shape that you observe visually. The reason is the same. You know when you do mathematical analysis and you ignore the physics of the problem in many engineering situations, you can make huge errors.

So, mathematical analysis should always be combined with scientific or engineering insight, and wherever possible, the science and engineering should actually take precedence over the mathematical analysis part.

Now, if the two are in complete agreement, that is fantastic but that very rarely happens, and so, you always have to decide where to give more weightage, and I think as engineers especially, we have to rely more on our engineering knowledge, experience, intuition in making decisions rather than basing them completely on mathematical analysis and whatever pops-out, right?

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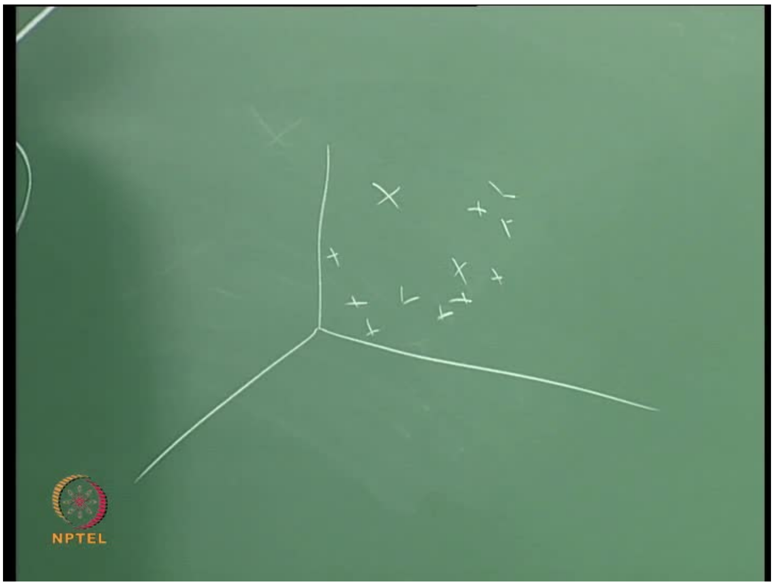

It's again the difference between, you know, c f t modeling and mechanistic modeling in a way. c f t modeling is very powerful, but you do not even some times physically understand what the model is telling you. Whereas mechanistic model may be much simpler, it may not capture all the complexities of the problem that c f t analysis does, but the result that comes from a mechanistic modeling will have more immediate relevance through an engineer, because it is, it is the analysis is based on the actual prevailing mechanism rather than trying to essentially force fit the data into a, you know, commercial package and accepting whatever comes out of it.

So, this is very similarly in shape analysis. You certainly have access to many tools, some of which are very sophisticated, but ultimately, you still have to rely more on your own physical insight into actually the first thing you should consider is the how the particle was generated in the first phase.

Do not treat the particle as a as a black box. Try to figure out first, what is the origination point? How did these particles come to exist in the first place? If it did it happen because of a phase change; it happened because of a mechanical process; did it happened because of a chemical reaction, because that level of insight or understanding can help you to homing in on the actual shape much faster than a completely empirical or mathematically based approach doing shape characterization. Ok.

So, I think with this lecture, we will complete our module on shape assessment, and from the next lecture onwards, we will move on to the second most important aspect of characters in particle morphology which is size characterization, but one point you should keep in mind is that the two are not really not separable. You cannot define shape without defining size and you cannot define size without defining shape.

And you know, it is like a chicken and the egg, what came first. Typically you do shape analysis first, because again, when the human eye encounters an object, the first thing it recognizes it is shape even before size. So, logically it makes sense to study shape first but the next most important aspect of an particle is its size, and so, we will spend a few lectures talking about size characterization in more detail. Any questions on what we have covered today? Ok. So, I will see you at the next lecture.