Dealing with Materials Data

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Lecture 56

Lorentz/Cauchy distribution

Welcome to Dealing with Materials Data in this course, we look at collection, analysis and interpretation of data from material science and engineering. We are specifically looking at probability distributions. And, we have looked at several discrete and continuous probability distributions. We are continuing with continuous probability distributions.

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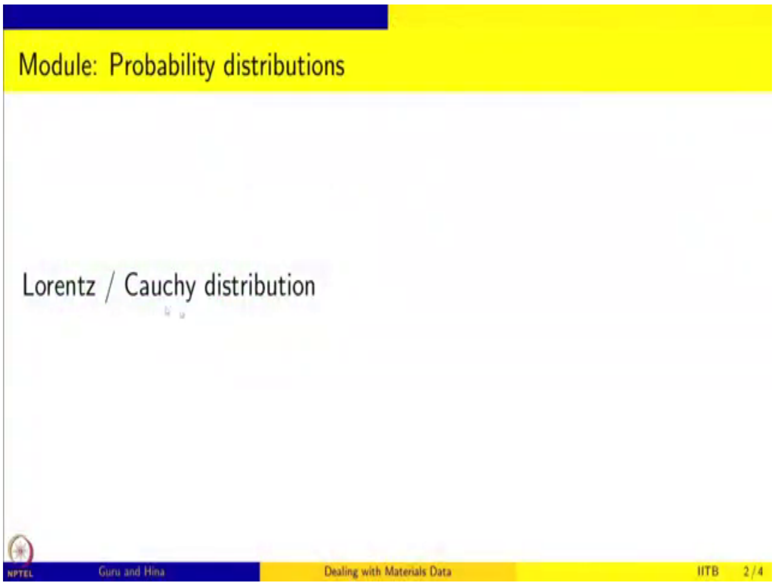

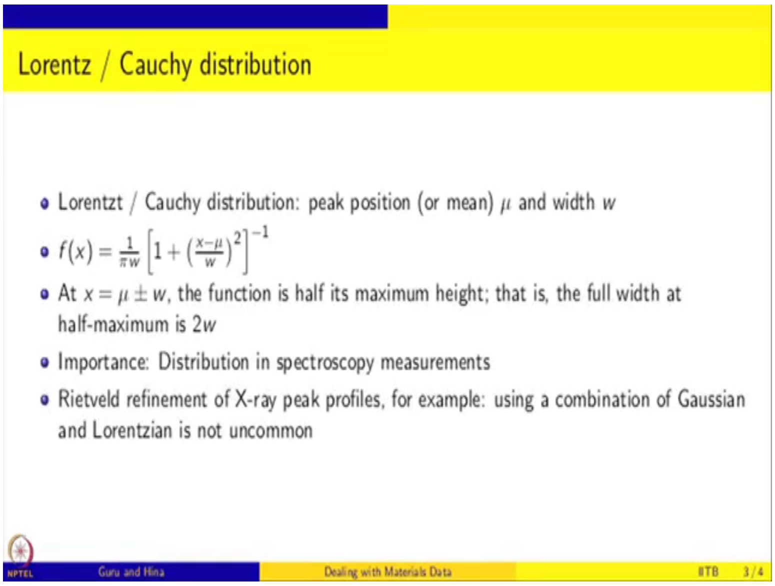

And, one of the important distributions which is important for in material science engineering is called a Lorentz distribution or Cauchy distribution. Lorentz or Cauchy distribution has 2 parameters, there is a peak position or mean, which is given by mu and there is a width w.

$$f(x) = \frac{1}{\pi w}\left[1 + (\frac{x-\mu}{w})^2\right]^{-1}$$

$$x = \mu \pm w$$

And, also when you do Rietveld refinement of X-ray peak profiles for example, it is not uncommon to see a combination of Gaussian and Lorentzian to fit the peak profiles. So, that is the reason why this is a very important distribution.

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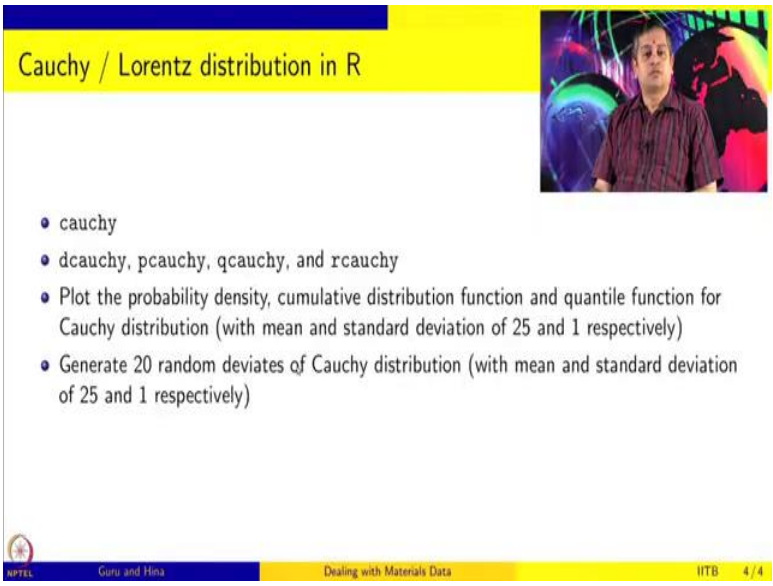

And, you can use Cauchy, dcauchy, pcauchy, qcauchy, rcauchy in R, to get the probability distribution function, cumulative distribution function, quantile function and random deviates. And, we will generate plots from the Cauchy distribution with the mean position at 25 and the width of 1 for example, and as usual we will plot and see what happens.

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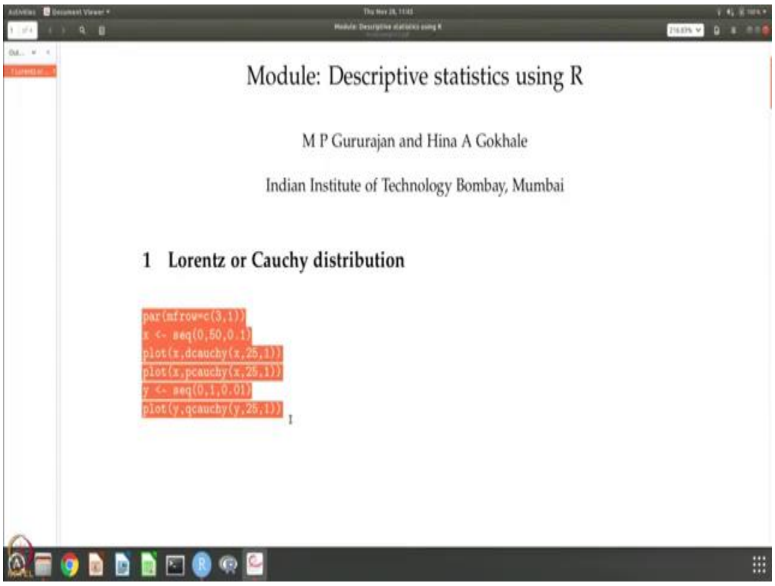

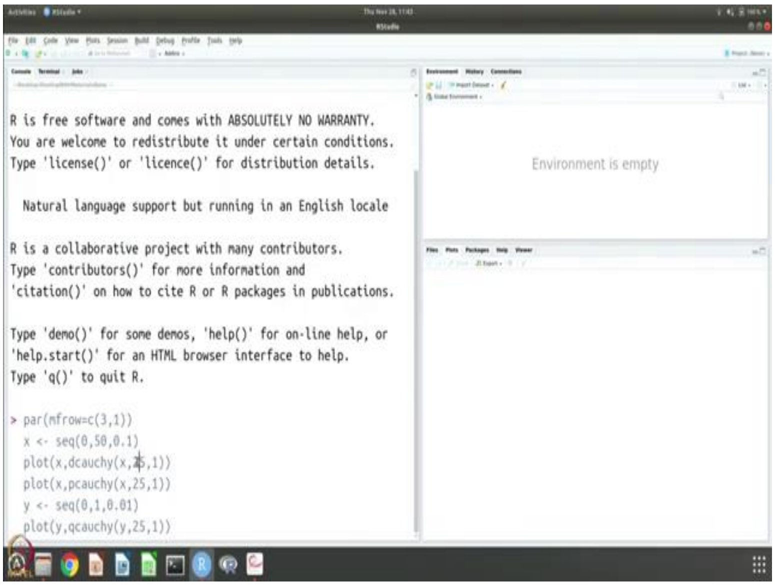

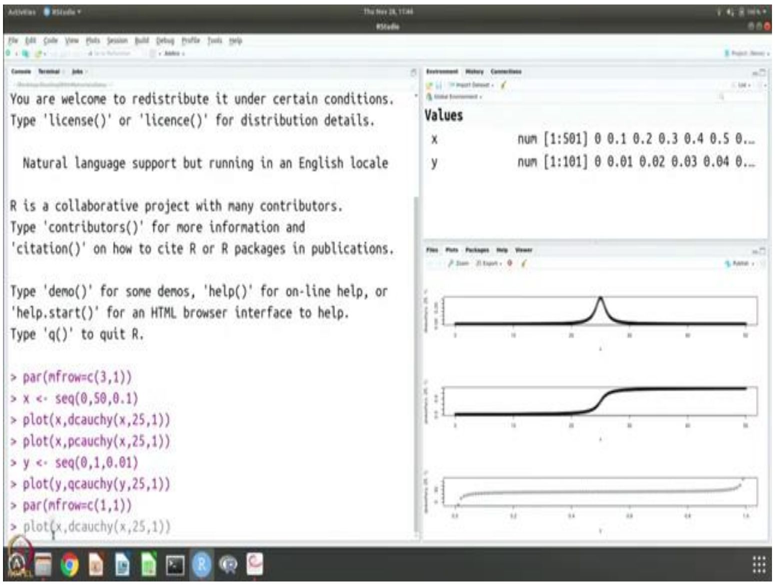

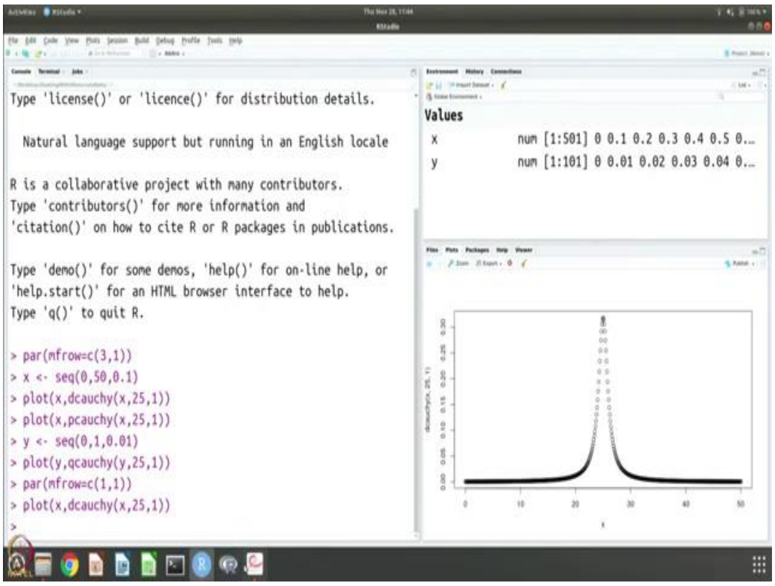

So, we are going to generate 3 plots, the first one is the probability distribution function, the second one is the cumulative distribution function and the third one is a quantile plot. And in all cases, we are going to use mean of 25 and width of 1. And so, this is how the Cauchy distribution function looks.

So, it must remind you of the spectroscopy or X-ray diffraction peaks that you typically tend to see. Of course, we can just plot the probability distribution function to see this better and so here is the plot. So, it looks very familiar I am sure because it looks like the peaks that you would see in some of these experiments.

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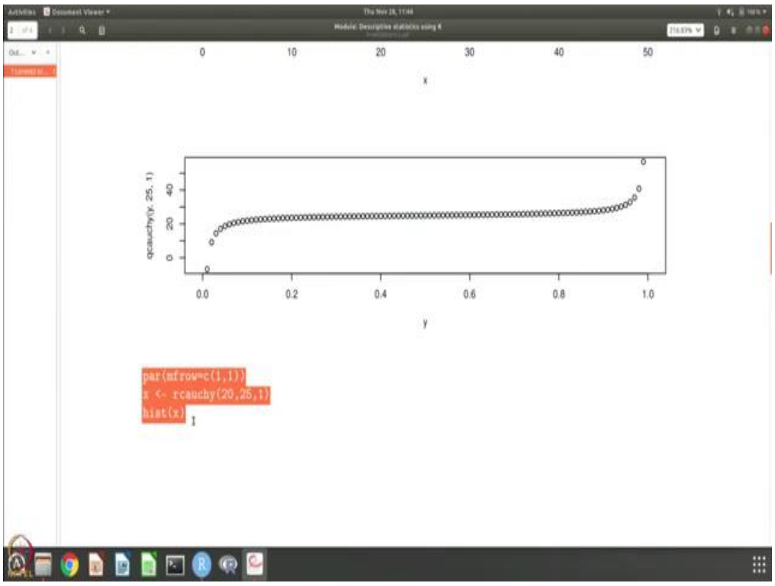

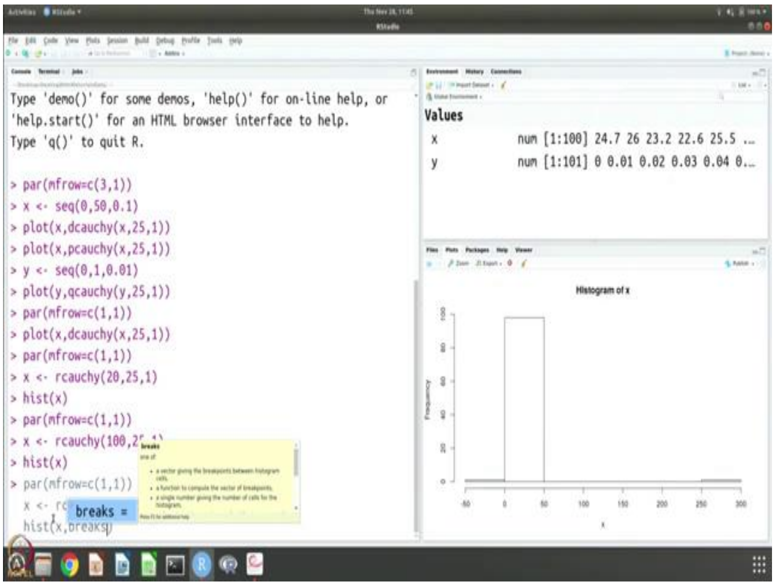

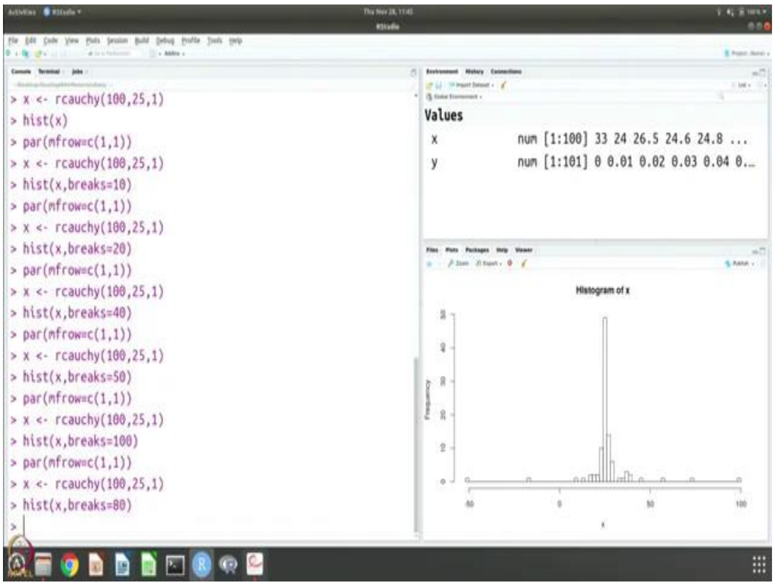

And of course, let us generate some random deviates and the plot the histogram that should also look very similar to this and so here you can see, maybe we should generate more deviates, so you can see or maybe we should need them more. Okay so you can now very clearly see the peak and it is at 25, it is expected at 25, so you can okay, so let us make, okay so, you can see that the data thus follow nice Cauchy distribution function.

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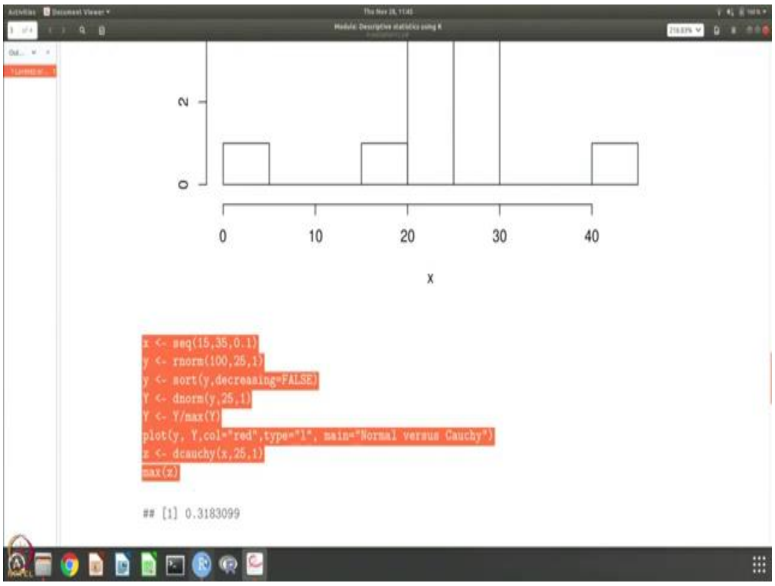

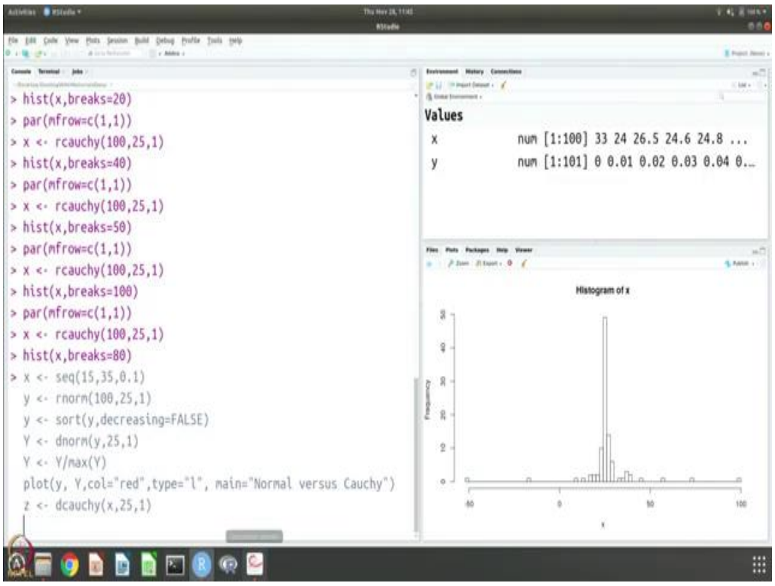

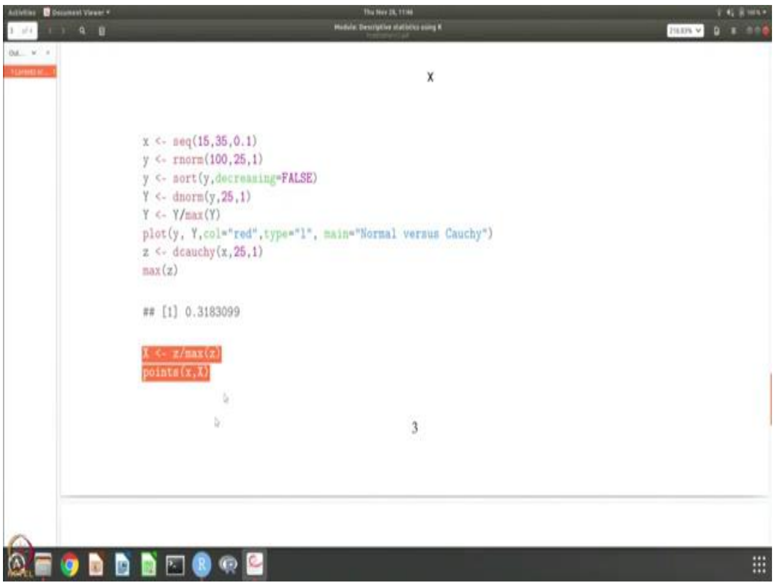

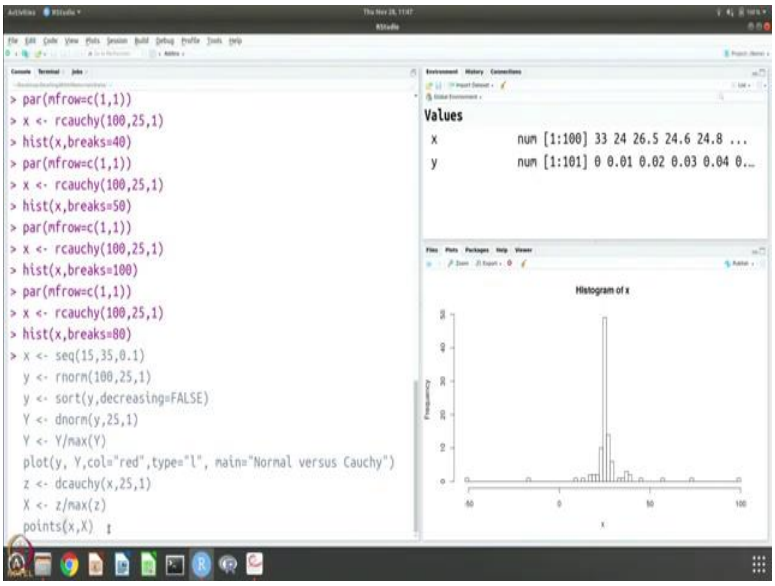

And there is one more exercise let us do, so how different is this distribution from normal distribution? So, we are going to do that, so let us understand what this script is doing. So, we take data points from 15 to 35 and we generate random deviates and we plot the data. But, we normalize the data so that the maximum will be 1 and that is what is done here.

So, random deviates and the probability distribution function using those random deviates after sorting, so that when you plot, it will give you a nice line and we plotted with red line. And then, we also generate random deviates from the probability distribution from the Cauchy distribution.

And notice that the normal and the Cauchy has the same mean and here it is the standard deviation here it is the width. Here again the Cauchy data is also normalized. So, that it will also peak at value of 1 and we are going to plot both. This is just to show you the deviation of Cauchy distribution from Gaussian, like I mentioned in Rietveld analysis, it is a combination of both which is used to describe the X-ray peaks.

So, it is a good idea to know how different they are from each other. So, we will plot it and see.

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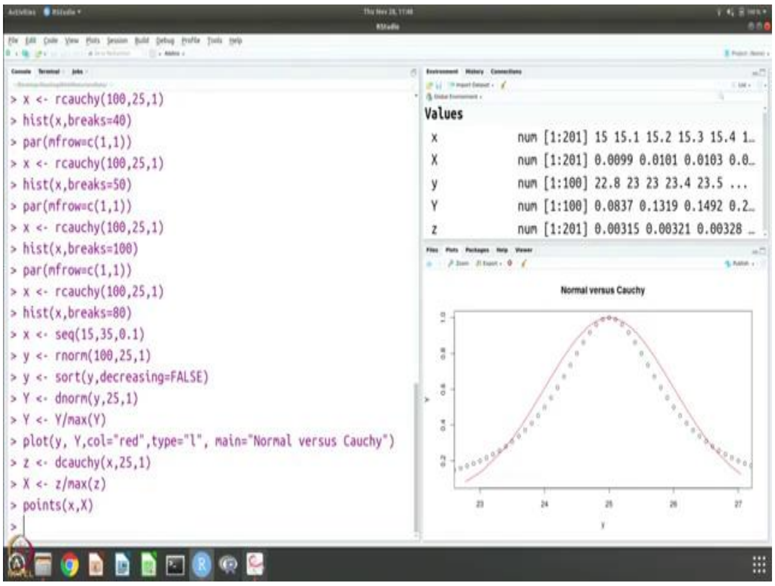

So, you can see the red line is the normal distribution. So, that is what, y is from the normal distribution and so, away from the peak, the Cauchy is still has some tail compared to the normal. Near the peak Cauchy is much more narrower than normal.

So, this is the difference between the two, so typical X-ray peak profiles are best described by a combination of two. There are other functions also that is used in ritual for refining the fitting of the peaks. But it is very common to see a combination of normal and Cauchy to fit. So, it is a good idea to know how they look and that is what we have done.

So, to conclude, Lorentz or Cauchy distribution is one of the common distributions, it is very important in material science engineering, because many experiments, spectroscopy experiments and like X-ray diffraction and such diffraction experiments, the peaks that if you want to fit, then Lorentz or Cauchy distribution is one of the important distributions that describe the shape of these peaks.

So, we have learned how to use R to generate random deviates as well as plot the probability distribution, cumulative distribution function and quantile functions as usual. So, the distribution is called Cauchy. It is not called Lorentz in R, so that is just a technical point that you have to remember. Thank you.