

Dealing with Materials Data: Collection, Analysis and Interpretation

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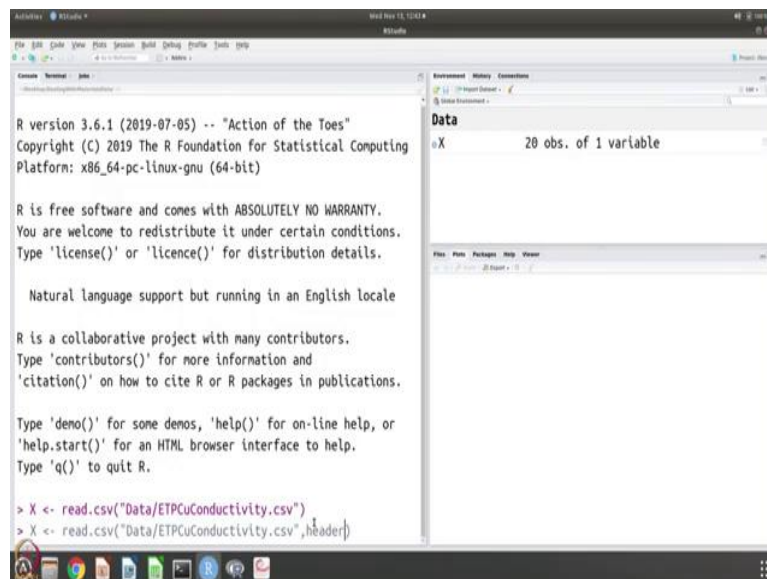
Indian Institute of Technology, Bombay

Lecture No. 21

Property based reports, errors, and significant digits

Welcome to Dealing with Materials Data. We are going to learn about Collection, Analysis and the Interpretation of materials data and we are doing module 2 which is for descriptive statistics using R. And, so we have been looking at preparing reports and we have looked at rank based and property based reports. So, let us concentrate on the property based reports a little bit more.

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R version 3.6.1 (2019-07-05) -- "Action of the Toes"
Copyright (C) 2019 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

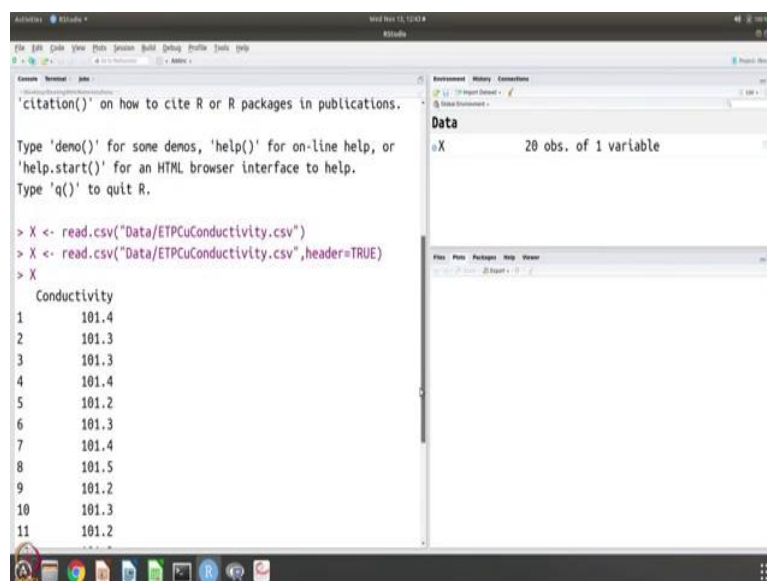
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Natural language support but running in an English locale

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> X <- read.csv("Data/ETPCuConductivity.csv")
> X <- read.csv("Data/ETPCuConductivity.csv",header)
```



```
'citation()' on how to cite R or R packages in publications.

Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> X <- read.csv("Data/ETPCuConductivity.csv")
> X <- read.csv("Data/ETPCuConductivity.csv",header=TRUE)
> X
  Conductivity
1      101.4
2      101.3
3      101.3
4      101.4
5      101.2
6      101.3
7      101.4
8      101.5
9      101.2
10     101.3
11     101.2
```

```

14      101.3
15      101.3
16      101.5
17      101.4
18      101.3
19      101.3
20      101.1

> x <- XSConductivity
> x
[1] 101.4 101.3 101.3 101.4 101.2 101.3 101.4 101.5 101.2
[10] 101.3 101.2 101.3 101.4 101.3 101.3 101.5 101.4 101.3
[19] 101.3 101.1
> mean(x)
[1] 101.32
> median(x)
[1] 101.3
> var(x)
[1] 0.01010526
> sd(x)
[1] 0.1005249
>

```

So, to do that we have been looking at this data on conductivity. So, let us read that file from data so this is data on Copper, ETP Copper electrical conductivity, electrolytic tough pitch copper conductivity. So, let us first read this information. So, it has 20 observations and 1 variable. So, there is this so it has a header so we say header is true. So, let us say X and it gives you this. And we have looked at this data in little bit have detail in the last session.

So, what we want to do? So, let us just store the conductivity data and this small x. So, these are all just numerical values so x now has just these numbers. Like I said, you can get the mean value of x, you get the median of x, you can get the variance of x. Variance is also called mean squared deviation and standard deviation is called root mean squared deviation. Now, as you can see the measurements of conductivity itself was reported only up to the first decimal place.

Because beyond this, the eddy current measurement cannot be accurate so. So, when we report the conductivity then we report the mean plus or minus standard deviation. So, typically it is reported this plus or minus standard deviation and here it is important not to report the result as 101.32 plus or minus 0.1005249. Because beyond this point the rest of the numbers do not make any sense.

Of course if you do an algebra you will get but the numbers themselves do not mean anything. So, we should take everything up to only the first decimal point or may be even less than that but at least you cannot report any value in the second decimal place that much is very clear.

It should be here or may be here but it cannot be anything beyond this point. So, the right way to report this number now the conductivity of this ETP Copper is 101.3 plus or minus 0.1. So,

this is called the significant digit beyond this digit the numbers have no significance, they do not have any meaning and we should not use them.

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Module: Descriptive statistics

Presenting experimental results: significant digits and error

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So, this is an important point and it is very crucial. So, we want to present experimental results and we need to understand significant digits and error when we present the results.

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Electrical conductivity of ETP copper

- 1 ETP: electrolytic tough pitch copper;
- 2 Conductivity measurement: eddy current method;
- 3 Units: % IACS (International Annealed Copper Standard);
- 4 Consider the data on copper conductivity;
- 5 Measurements carried out by Dr N Harshavardhana, and reported in his PhD thesis submitted to IITB.

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So, again this is ETP Copper and the measurement is in terms of IACS.

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ETP copper: conductivity data

101.4	101.3	101.3	101.4	101.2
101.3	101.4	101.5	101.2	101.3
101.2	101.3	101.4	101.3	101.3
101.5	101.4	101.3	101.3	101.1

20 measurements of ETP copper using eddy current method; the values are in % IACS.
Data stored in ETPCuConductivity.csv


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And these are the numbers.

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Property based reports

- Mean: 101.32
- Median: 101.2
- Standard deviation: 0.1005249 (Root mean squared deviation – RMSD)
- Variance: 0.01010526 (Mean-squared-deviation – MSD)
- Significant digits: Since the conductivity measurements themselves are only reported upto the first decimal place, it does not make sense to report the mean and standard deviation beyond that!
- Mean: 101.3
- Standard deviation: 0.1
- Conductivity: 101.3 ± 0.1 % IACS

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And what we did is to calculate the mean, median, standard deviation and variance. And standard deviation is called root mean squared deviation - RMSD and variance is called mean squared deviation - MSD. And because all the conductivity measurements are reported up to first decimal place. The mean and standard deviation also should be reported only up to this or less than this it cannot be more than that.

So, mean is 101.3, standard deviation is 0.1. So, the right way to report conductivity for this Copper sample is 101.3 plus or minus 0.1 percentage IACS. And because we have seen that in

the case of this conductivity data, the data seems to be a normal distribution. So, giving mean and the standard deviation is sufficient to completely describe the information.

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Errors reporting

- It is better to be conservative in error estimation: that is, if the calculations give a number of 1.475 for error, round it up to 2 instead of rounding it down to 1.
- Inaccuracies can be expressed as absolute values like we did earlier: conductivity is 101.3 ± 0.1 % IACS
- You can also report it as a relative quantity: Conductivity: $101.3 \pm 0.1\%$

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Property based reports

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- Variance: 0.01010526 (Mean-squared-deviation – MSD)
- Significant digits: Since the conductivity measurements themselves are only reported upto the first decimal place, it does not make sense to report the mean and standard deviation beyond that!
- Mean: 101.3
- Standard deviation: 0.1
- Conductivity: 101.3 ± 0.1 % IACS

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And there is one more point in terms of reporting the errors. So, we have reported the error as 0.1 so that is in terms of the value itself. So, this 0.1 also has the unit of percentage of IACS. But, you can also report it as a percentage itself, you can report 101.3 percentage IACS plus or minus 0.1 percent. There should be no confusion that 0.1 just becomes 0.1 percent that is not the case and this percentage is with percentage IACS, it is with the unit. If you take 0.1 and divide by 101.3 that also happens to be 0.1 percent and that is why it is reported as a relative quantity as 0.1 percent.

So, it is 101.3 plus or minus 0.1 percent, percent IACS is the correct way of reporting. So, the error can be reported in both ways as an absolute error or as a relative error and you can do either way. And one more point that we have to remember is that, it is better to be conservative in error estimation.

If your calculations give some number like 1.475 for error we should put it up as 2 instead of rounding down to 1. 1.475 so it is better to call it as 2 even though you might think that 1.4 or even if it is 1.375 for example, which makes it 1.4. We should still report it as 2.

This is just to be conservative. We are not saying that so if you actually round it off. It should be 1.1 say but even then if it is an error, if you want to be conservative about error estimates, you should always round it up instead of rounding it down so it is a good practice. So, this is about significant digits and error, we will do more of the analysis on errors later. This is just in terms of reporting the observed values.

So, we will take a look at slightly more involved data, so we just looked at one property measurement which is conductivity and we found that 20 measurements gives some the numbers and from there we prepared some reports on the rank based and property based values for this data. But, we can do it for more complicated data also.

So, we are going to next consider another sort of measurement that is very-very common in material science. But, it is slightly different in terms of how we measure these quantities. So, we are going to discuss that in greater detail in the next session. Thank you.