## Introduction to Scientific Computation



Halil Bayraktar
Lecture 7-data normalization, missing values and functions in programming

## How to clean missing values in the data?



## Solution 1:

## We can use the rmmissing function that removes all rows with NaN

|  |  | $\begin{gathered} 30 \\ \text { TRNA13 } \end{gathered}$ | $\begin{gathered} 31 \\ \text { TRNA14 } \end{gathered}$ | $\begin{gathered} 32 \\ \text { Young_vs_Old } \end{gathered}$ | $\begin{gathered} 33 \\ \text { Old_vs_AD } \end{gathered}$ | $\begin{gathered} 34 \\ \text { Young_vs_AD } \end{gathered}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 16 | 2.5888 | 0.9477 | NaN | 0.6577 | 0.9316 |
| ! | '4 | 28.4767 | 37.9071 | 0.2173 | 0.9606 | 0.1592 |
| ) | 0 | 0 | 0 | NaN | NaN | NaN |
| + | '9 | 11.2181 | 36.9594 | 0.7778 | 0.4949 | 0.2141 |
| ; | 15 | 134.6172 | 93.8201 | 0.2529 | 0.5152 | 0.0180 |
| ; | 0 | 0 | 0 | NaN | NaN | NaN |
| ' | 37 | 217.4585 | 149.7331 | 0.8257 | 0.0248 | 0.0035 |
| ; | 34 | 225.2249 | 373.3850 | 0.8962 | 0.1639 | 0.0661 |
| 1 | 0 | 0 | 0 | NaN | NaN | NaN |
| 10 | 0 | 0 | 4.7384 | NaN | 0.0820 | 0.4243 |
| \|1 | 0 | 0 | 0.9477 | NaN | NaN | NaN |
| 12 | 15 | 356.3903 | 397.0770 | 0.6785 | 0.7987 | 0.3801 |
| 13 | 13 | $1.2452 \mathrm{e}+03$ | $1.4860 \mathrm{e}+03$ | 0.8661 | 0.9385 | 0.7631 |
| 14 | 13 | $1.6439 \mathrm{e}+03$ | $1.5068 \mathrm{e}+03$ | 0.4814 | 0.2136 | 0.0121 |
| 15 | 0 | 1.7259 | 1.8954 | NaN | 0.3701 | 0.0193 |
| 16 | 34 | 220.0473 | 470.9958 | 0.3814 | 0.3493 | 0.9747 |
| 17 | '8 | 739.5315 | 273.8789 | 0.3138 | 0.7563 | 0.0845 |
| 18 | 37 | 43.1465 | 71.0758 | 0.1019 | 0.7264 | 0.1319 |
| 19 | 0 | 0 | 0 | NaN | NaN | NaN |
| $!0$ | 0 | 0 | 1.8954 | NaN | NaN | NaN |
| ! 1 | 13 | $1.1926 \mathrm{e}+03$ | 981.7941 | 0.5825 | 0.8988 | 0.3862 |
| $!2$ | 13 | $1.4256 \mathrm{e}+03$ | $1.1903 \mathrm{e}+03$ | 0.3570 | 0.9632 | 0.2343 |
| 13 | j0 | 73.3491 | 60.6514 | 0.6285 | 0.2586 | 0.0371 |
| $!4$ | 24 | 46.5983 | 49.2792 | 0.8579 | 0.3470 | 0.1649 |


| $\boxplus 128 \times 33$ double |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 27.8394 | 37.1676 | 55.2547 | 30.2348 | 42.7112 | 32.2643 |
| 2 | 41.2024 | 35.1586 | 40.1853 | 16.4917 | 35.7582 | 32.2643 |
| 3 | 111.3578 | 123.5573 | 118.5465 | 133.7663 | 91.3821 | 86.7800 |
| 4 | 190.4218 | 183.8291 | 141.6531 | 169.4984 | 155.9455 | 92.3428 |
| 5 | 259.4637 | 291.3139 | 188.8708 | 237.2977 | 289.0455 | 189.1358 |
| 6 | 485.5200 | 435.9663 | 492.2695 | 308.7619 | 511.5410 | 493.9782 |
| 7 | $1.1559 \mathrm{e}+03$ | $1.0035 \mathrm{e}+03$ | $1.2116 \mathrm{e}+03$ | $1.3138 \mathrm{e}+03$ | $1.3479 \mathrm{e}+03$ | $1.4652 \mathrm{e}+03$ |
| 8 | $1.2550 \mathrm{e}+03$ | $1.8232 \mathrm{e}+03$ | $1.3914 \mathrm{e}+03$ | $1.4861 \mathrm{e}+03$ | $1.5545 \mathrm{e}+03$ | $1.3206 \mathrm{e}+03$ |
| 9 | 780.6181 | 676.0491 | 640.9550 | 244.6274 | 522.4672 | 406.0857 |
| 10 | 309.5747 | 294.3275 | 372.7184 | 721.0553 | 238.3881 | 354.9078 |
| 11 | 113.5849 | 91.4123 | 74.3427 | 89.7883 | 100.3216 | 160.2091 |
| 12 | $1.3274 \mathrm{e}+03$ | $1.6374 \mathrm{e}+03$ | $1.3000 \mathrm{e}+03$ | $1.2341 \mathrm{e}+03$ | $1.2416 \mathrm{e}+03$ | $1.4953 \mathrm{e}+03$ |
| 13 | $1.3285 \mathrm{e}+03$ | 1.1422e+03 | 977.5067 | 1.1333e+03 | $1.3072 \mathrm{e}+03$ | $1.1738 \mathrm{e}+03$ |
| 14 | 150.3330 | 145.6569 | 190.8800 | 127.3528 | 113.2343 | 140.1830 |
| 15 | 66.8147 | 36.1631 | 46.2131 | 39.3969 | 31.7851 | 52.2905 |
| 16 | 153.6738 | 171.7747 | 161.7457 | 154.8391 | 164.8851 | 141.2956 |
| 17 | 146.9923 | 150.6796 | 110.5095 | 95.2856 | 85.4224 | 74.5418 |
| 18 | 197.1033 | 381.7216 | 150.6948 | 362.8182 | 73.5030 | 70.0915 |
| 19 | 20.0444 | 12.0544 | 21.0973 | 6.4135 | 20.8590 | 66.7538 |
| 20 | $1.4610 \mathrm{e}+03$ | 747.3707 | 816.7656 | 209.8115 | 345.6627 | 269.2404 |
| 21 | 228.2835 | 198.8971 | 337.5563 | 285.8567 | 128.1336 | 133.5076 |

## Solution 2:

Can we write our own code that removes the data with zeros?
How to find Nan values in the data and remove these arrays?


## Data normalization

1. Divide by the max value or
2. Find largest of smallest value and use the following formula, you can scale the values between 0 and 1

Data-min/max-min

$$
x^{\prime}=\left(x-x_{\min }\right) /\left(x_{\max }-x_{\min }\right)
$$

```
%%
data1=randi([10,100],10,5)
%%
mad=max(max(data1))
mid=min(min(data1))
ndata=(data1-mid)/(mad-mid)
```

|  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | 10x5 double


| T10x5 double |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 0.8652 | 0.6292 | 0.7191 | 0.1124 | 0.0787 |  |
| 2 | 0.0562 | 0.4045 | 0.7978 | 0.7978 | 0.4607 |  |
| 3 | 0.3596 | 0.3596 | 0.5730 | 0.4607 | 0.7865 |  |
| 4 | 0.2584 | 0.6517 | 0.0225 | 0.3034 | 0.8315 |  |
| 5 | 0.4382 | 0.7416 | 0 | 0.3596 | 0.6404 |  |
| 6 | 0.3034 | 0.7416 | 1 | 0.4831 | 0.3708 |  |
| 7 | 0.9775 | 0.9775 | 0.2022 | 0.4382 | 0.8989 |  |
| 8 | 0.1236 | 0.0449 | 0.8315 | 0.7079 | 0.2472 |  |
| 9 | 0.2135 | 0.4270 | 0.3596 | 0.6854 | 0.0674 |  |
| 10 | 0.9101 | 0 | 0.4607 | 0 | 0.7416 |  |
| 11 |  |  |  |  |  |  |
| 12 |  |  |  |  |  |  |

## Log scaling

It is used to scae the values and compress a wide range to a narrow range of values.



```
%%
%log scaling
% example
clear y
x=1:1:400
for i=1:400
    y(1,i)=20000/exp(0.02*x(1,i))
end
figure(1)
subplot(1,2,1)
bar(x,y)
ylabel('y')
set(gca,'fontsize',24)
subplot(1,2,2)
bar(x,log10(y))
ylabel('log10(y)')
set(gca,'fontsize',24)
```


## Subgrouping the data

\% mean values of each gene for young, old, and AD samples allmeansdata=subyoungmean'; allmeansdata(: $; 2$ )=suboldmean'; allmeansdata(: $: 3$ )=subADmean';
\% young old diff
allmeansdata(:, 4)= allmelansdata (: 1)- allmeansdata (:, 2); \% young alz diff
allmeansdata(:, 5)= allmeansdata (: 1)- allmeansdata (:, 3); \% old alzhemier diff
allmeansdata(:, 6)= allmeansdata (:, 2)- allmeansdata (: $: 3$ );

| $\boxplus 128 \times 11$ double |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 0.4866 | 0.6443 | 0.6451 | -0.1577 | -0.1585 | -8.7756e-04 |
| 2 | 0.5456 | 0.6937 | 0.6966 | -0.1481 | -0.1510 | -0.0029 |
| 3 | 0.2530 | 0.4804 | 0.4837 | -0.2274 | -0.2307 | -0.0033 |
| 4 | 0.6238 | 0.7190 | 0.7131 | -0.0952 | -0.0893 | 0.0059 |
| 5 | 0.6202 | 0.4621 | 0.4699 | 0.1581 | 0.1504 | -0.0077 |
| 6 | 0.7676 | 0.6858 | 0.6771 | 0.0818 | 0.0905 | 0.0087 |
| 7 | 0.8241 | 0.6859 | 0.6761 | 0.1382 | 0.1480 | 0.0098 |
| 8 | 0.4072 | 0.5010 | 0.4909 | -0.0938 | -0.0837 | 0.0101 |
| 9 | 0.3752 | 0.4150 | 0.4031 | -0.0398 | -0.0279 | 0.0119 |
| 10 | 0.5472 | 0.6547 | 0.6675 | -0.1075 | -0.1202 | -0.0127 |
| 11 | 0.7443 | 0.6082 | 0.6215 | 0.1361 | 0.1229 | -0.0132 |
| 12 | 0.6721 | 0.5565 | 0.5408 | 0.1157 | 0.1314 | 0.0157 |
| 13 | 0.6649 | 0.5888 | 0.6067 | 0.0761 | 0.0581 | -0.0180 |
| 14 | 0.4952 | 0.3110 | 0.3305 | 0.1843 | 0.1647 | -0.0196 |
| 15 | 0.8474 | 0.7785 | 0.8004 | 0.0689 | 0.0470 | -0.0219 |
| 16 | 0.4533 | 0.6328 | 0.6089 | -0.1795 | -0.1556 | 0.0239 |
| 17 | 0.7804 | 0.6416 | 0.6657 | 0.1388 | 0.1147 | -0.0241 |
| 18 | 0.5196 | 0.5083 | 0.5332 | 0.0113 | -0.0136 | -0.0250 |
| 19 | 0.3145 | 0.3653 | 0.3352 | -0.0508 | -0.0207 | 0.0301 |
| 20 | 0.5720 | 0.5746 | 0.6052 | -0.0026 | -0.0332 | -0.0306 |
| 21 | 0.6814 | 0.6760 | 0.6448 | 0.0054 | 0.0367 | 0.0313 |
| - |  |  |  | n moa |  | 0 nonr |

## IF statement

If statement is used to choose whether or not a statement, or group of statements, is executed. if statement is written as,

If logic expression or relational expression arguments
elseif logic or relational expression Arguments
end
end

## Switch Statement

A switch statement can often be used in place of a nested if-else or an if statement with many elseif clauses.
Switch statements are used when an expression is tested to see whether it is equal to one of several possible values.

## switch switch_expression

case caseexp1 action1
case caseexp2 action2
case caseexp3 action3
\% etc: there can be many of these otherwise actionn end

## Numeric values as a case

```
month=input('select a month:')
switch month
    case {1,3,5,7,8,10,12} % group different case varibles if return same results
        days=31;
        fprintf('days: %i',days)
    case {4,6,9,11}
        days=30
        fprintf('days: %i',days)
    case 2
        days=28
        fprintf('days: %i',days)
    otherwise
        disp('entered valuer is not present, please select a number between 1 and 12')
end
```


## String values as a case

```
%% enter a string
% if and case statements
food=input('enter a food: ')
switch food
    case {'pizza','burger','chips'}
        disp('food is not healthy')
    case {'soup','vegetable','rice'}
        disp('food is healthy')
        if food=='soup'
        disp('soup has high protein nutrients')
        else
        disp('it has high carbohydrate nutrient')
        end
    otherwise
        disp('i do not know')
end
```


## Create a menu tab in the matlab

```
%% menu in matlab
degree=input('enter a angle in degrees: ')
choice=menu('function','sin','cos','tan','cot')
switch choice
    case {1}
        result=sind(degree)
    case {2}
        result=cosd(degree)
    case {3}
    result=tand(degree)
    case {4}
        result=cotd(degree)
end
fprintf('%i',result)
```


result $=$
0.5000

$f$| $f \times 5.000000 \mathrm{e}-01 \gg$ | $\square$ |
| :--- | :--- |

## Is Functions in Matlab

```
%% is functions In Matlab
isnumeric(56)
%%
isletter('334678888 Maslak')
%%
y=[
x=[1,2,3]
isempty(y)
x=45
isstring(x)
%%
isnumeric(34)
%%
a=[1,2]
isempty(a)
a=["maslak"]
isstring(a)
isletter('a')
a=[1,2]
isempty(a)
isreal(0)
%%
a=[1,2,3,NaN]
find(ISnan(a))
```


## How to write a function in Matlab

function [output value 1, output value 2, ...] =name(input1, input2,input3...])
body of the function
end

```
    function [result]=name(x,y,z,......)
    % function to compute the factorial of a number
    body of the function
    end
```


## Any matlab function consists of

1. Each function in the matlab starts with a word of "function", please do not use this word any other place in your code.
2. Find a name for your function (note: The name should be the same as the name of the M-file in which this function is stored)
3. The input values are shown in parentheses. They are separated by commas if there is more than one input values.
4. Output values are shown in square brackets. If there are more than one inputs, they are separated by comma.

Example: Function to compute the factorial of a number function [fac]=factfun(n)
\% function to compute factorial of a number

```
fac=1;
for \(\mathrm{i}=1: \mathrm{n} ;\)
    fac=fac*;
```

end
format short
\%result=fac;
fprintf('\%i factorial equals to \%i $\backslash n ', n, f a c)$

## Example: Function to compute the factorial of a number

function [fac]=factfun2(n)
\% function to compute factorial of a number
if $\mathrm{n}==0$
$f a c=1$
fprintf('\%i factorial equals to \%i $\backslash n ', n, f a c)$ return
else
fac=prod(1:n)
end
format short
\%result=fac;
fprintf('\%i factorial equals to \%i $\backslash n ', n, f a c)$
fprintf('it works')
end

## Anonymous Functions

Anonymous functions are functionsdefine d in your program.
it does not need other file to save it. We use a symbol of @
@(input variable) expression
quad function in matlab evaluates the integration of a function between two values.

$$
\begin{gathered}
a=@(x) \sin (x) .{ }^{*} \cos (x) ; \\
\text { quad }(a, 0,3)
\end{gathered}
$$

$$
\text { Ans }=0.01
$$

$$
\begin{aligned}
& I=\frac{2}{2} \int \sin x \cos x d x \\
& I=\frac{1}{2} \int 2 \sin x \cos x d x \\
& I=\frac{1}{2} \int \sin 2 x d x \\
& I=-\frac{1}{2} \frac{\cos 2 x}{2} \\
& I=\frac{-\cos 2 x}{4}+C \\
& \hline
\end{aligned}
$$

## Examples of Anonymous Functions

$$
\begin{gathered}
\text { sqr }=@(x) x .^{\wedge} 2 ; \\
a=\operatorname{sqr}(5)
\end{gathered}
$$

function1=@(x,y,z) x.^2+y.^3+z.^4 function1(1,2,3)
function1 =
function_handle with value:

$$
@(x, y, z) x .^{\wedge} 2+y .^{\wedge} 3+z .^{\wedge} 4
$$

ans =
90

