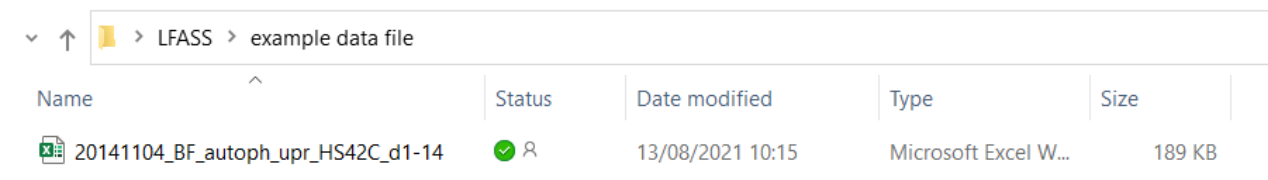


1. Download and install Matlab (Mathworks).
2. Download and copy LFASS folder where needed (<https://github.com/ABA80/LFASS>).
3. Open LFASS folder:

LFASS				
Name	Status	Date modified	Type	Size
fitfolder	✓ ⓘ	28/01/2022 17:06	MATLAB Code	17 KB
Save_after_refit_crash	✓ ⓘ	30/12/2021 14:22	MATLAB Code	1 KB
fitc	✓ ⓘ	29/12/2021 21:20	MATLAB Code	7 KB
user_basicfunc	✓ ⓘ	23/11/2017 15:20	MATLAB Code	3 KB
plotalc	✓ ⓘ	23/11/2017 15:20	MATLAB Code	2 KB
testfit	✓ ⓘ	23/11/2017 15:20	MATLAB Code	8 KB
user_fitc	✓ ⓘ	23/11/2017 15:20	MATLAB Code	9 KB
isnoise	✓ ⓘ	23/11/2017 15:20	MATLAB Code	2 KB
modelfunc	✓ ⓘ	23/11/2017 15:20	MATLAB Code	1 KB
plotal	✓ ⓘ	23/11/2017 15:20	MATLAB Code	2 KB
fitctag	✓ ⓘ	23/11/2017 15:20	MATLAB Code	10 KB
analyses	✓ ⓘ	23/11/2017 15:20	MATLAB Code	2 KB
basicfunc	✓ ⓘ	23/11/2017 15:20	MATLAB Code	3 KB
analyse	✓ ⓘ	23/11/2017 15:20	MATLAB Code	8 KB
results_folder	✓ ⓘ	15/03/2022 15:03	File folder	
data	✓ ⓘ	15/03/2022 14:56	File folder	
example data file	✓ ⓘ	13/08/2021 10:15	File folder	
Guide for LFASS users	✓ ⓘ	09/11/2020 09:56	File folder	

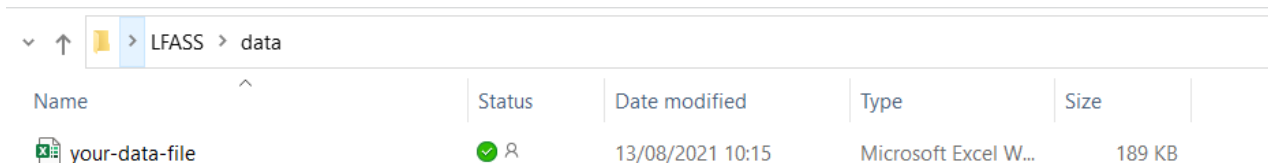
4. 'results_folder' may not be there. It will be automatically created when running the routine for the first time.

5. You can use the file in the 'example data' folder to practice:



Name	Status	Date modified	Type	Size
20141104_BF_autoph_uvr_HS42C_d1-14	✓	13/08/2021 10:15	Microsoft Excel W...	189 KB

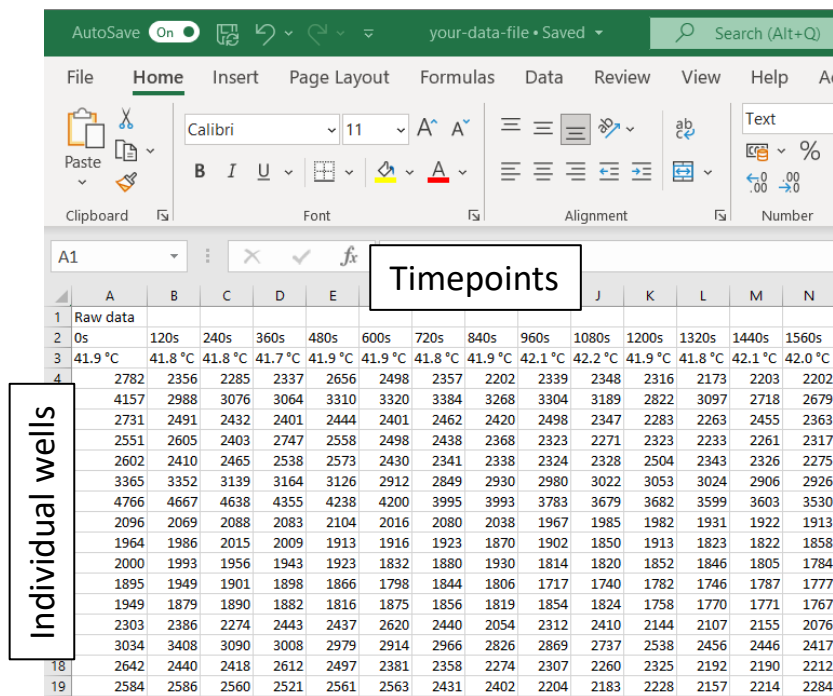
6. Copy it in the 'data' folder, or copy your own data file:



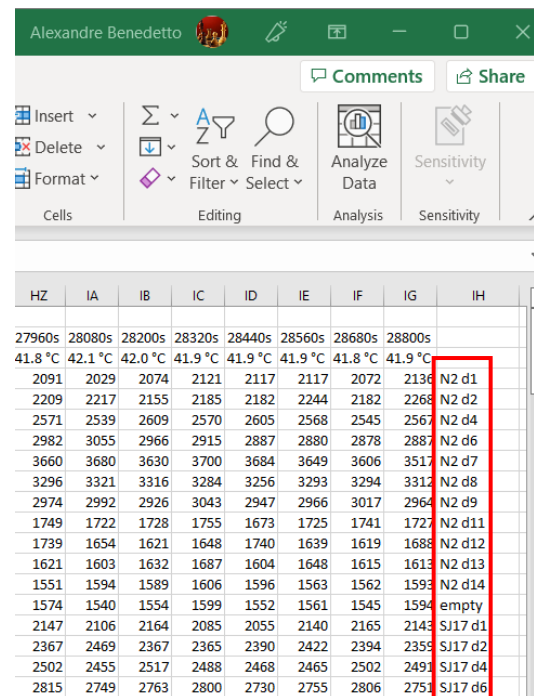
Name	Status	Date modified	Type	Size
your-data-file	✓	13/08/2021 10:15	Microsoft Excel W...	189 KB

7. Your data file should be organised as follows:

- Wells in rows
- Timepoints in columns
- Identifiers for wells in first or last column
- Non-number rows (headings, temperatures) will be ignored



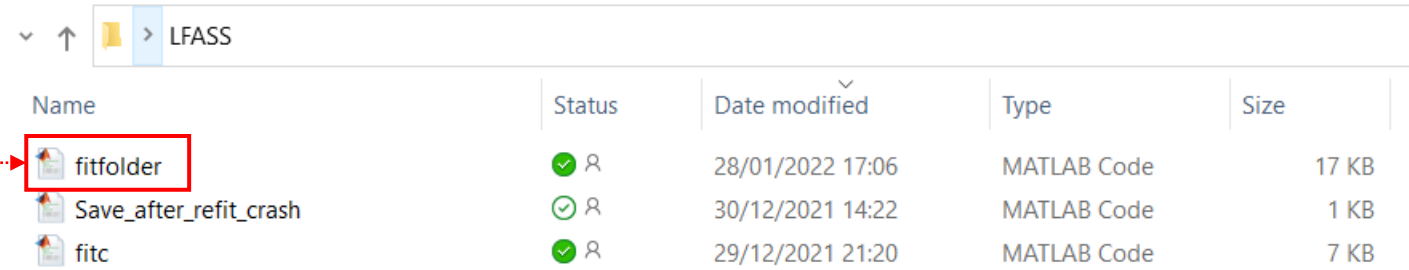
	A	B	C	D	E	F	G	H	I	J	K	L	M	N
1	Raw data													
2	0s	120s	240s	360s	480s	600s	720s	840s	960s	1080s	1200s	1320s	1440s	1560s
3	41.9 °C	41.8 °C	41.8 °C	41.7 °C	41.9 °C	41.9 °C	41.8 °C	41.9 °C	42.1 °C	42.2 °C	41.9 °C	41.8 °C	42.1 °C	42.0 °C
4	2782	2356	2285	2337	2656	2498	2357	2202	2339	2348	2316	2173	2203	2202
5	4157	2988	3076	3064	3310	3320	3384	3268	3304	3189	2822	3097	2718	2679
6	2731	2491	2432	2401	2444	2401	2462	2420	2498	2347	2283	2263	2455	2363
7	2551	2605	2403	2747	2558	2498	2438	2368	2323	2271	2323	2233	2261	2317
8	2602	2410	2465	2538	2573	2430	2341	2338	2324	2328	2504	2343	2326	2275
9	3365	3352	3139	3164	3126	2912	2849	2930	2980	3022	3053	3024	2906	2926
10	4766	4667	4638	4355	4238	4200	3995	3993	3783	3679	3682	3599	3603	3530
11	2096	2069	2088	2083	2104	2016	2080	2038	1967	1985	1982	1931	1922	1913
12	1964	1986	2015	2009	1913	1916	1923	1870	1902	1850	1913	1823	1822	1858
13	2000	1993	1956	1943	1923	1832	1880	1930	1814	1820	1852	1846	1805	1784
14	1895	1949	1901	1898	1866	1798	1844	1806	1717	1740	1782	1746	1787	1777
15	1949	1879	1890	1882	1816	1875	1856	1819	1854	1824	1758	1770	1771	1767
16	2303	2386	2274	2443	2437	2620	2440	2054	2312	2410	2144	2107	2155	2076
17	3034	3408	3090	3008	2979	2914	2966	2826	2869	2737	2538	2456	2446	2417
18	2642	2440	2418	2612	2497	2381	2358	2274	2307	2260	2325	2192	2190	2212
19	2584	2586	2560	2521	2561	2563	2431	2402	2204	2183	2228	2157	2214	2284



HZ	IA	IB	IC	ID	IE	IF	IG	IH
27960s	28080s	28200s	28320s	28440s	28560s	28680s	28800s	
41.8 °C	42.1 °C	42.0 °C	41.9 °C	41.9 °C	41.9 °C	41.8 °C	41.9 °C	
2091	2029	2074	2121	2117	2072	2136	N2 d1	
2209	2217	2155	2185	2182	2244	2182	N2 d2	
2571	2539	2609	2570	2605	2568	2545	N2 d4	
2982	3055	2966	2915	2887	2880	2878	N2 d6	
3660	3680	3630	3700	3684	3649	3606	N2 d7	
3296	3321	3316	3284	3256	3293	3294	N2 d8	
2974	2992	2926	3043	2947	2966	3017	N2 d9	
1749	1722	1728	1755	1673	1725	1741	N2 d11	
1739	1654	1621	1648	1740	1639	1619	N2 d12	
1621	1603	1632	1687	1604	1648	1615	N2 d13	
1551	1594	1589	1606	1596	1563	1562	N2 d14	
1574	1540	1554	1599	1552	1561	1545	empty	
2147	2106	2164	2085	2055	2140	2165	SJ17 d1	
2367	2469	2367	2365	2390	2422	2394	SJ17 d2	
2502	2455	2517	2488	2468	2465	2502	SJ17 d4	
2815	2749	2763	2800	2730	2755	2806	SJ17 d6	

Well identifiers / labels

8. Double-click on the 'fitfolder' file in the LFASS folder (it will open Matlab automatically)




Name	Status	Date modified	Type	Size
fitfolder	✓	28/01/2022 17:06	MATLAB Code	17 KB
Save_after_refit_crash	✓	30/12/2021 14:22	MATLAB Code	1 KB
fitc	✓	29/12/2021 21:20	MATLAB Code	7 KB

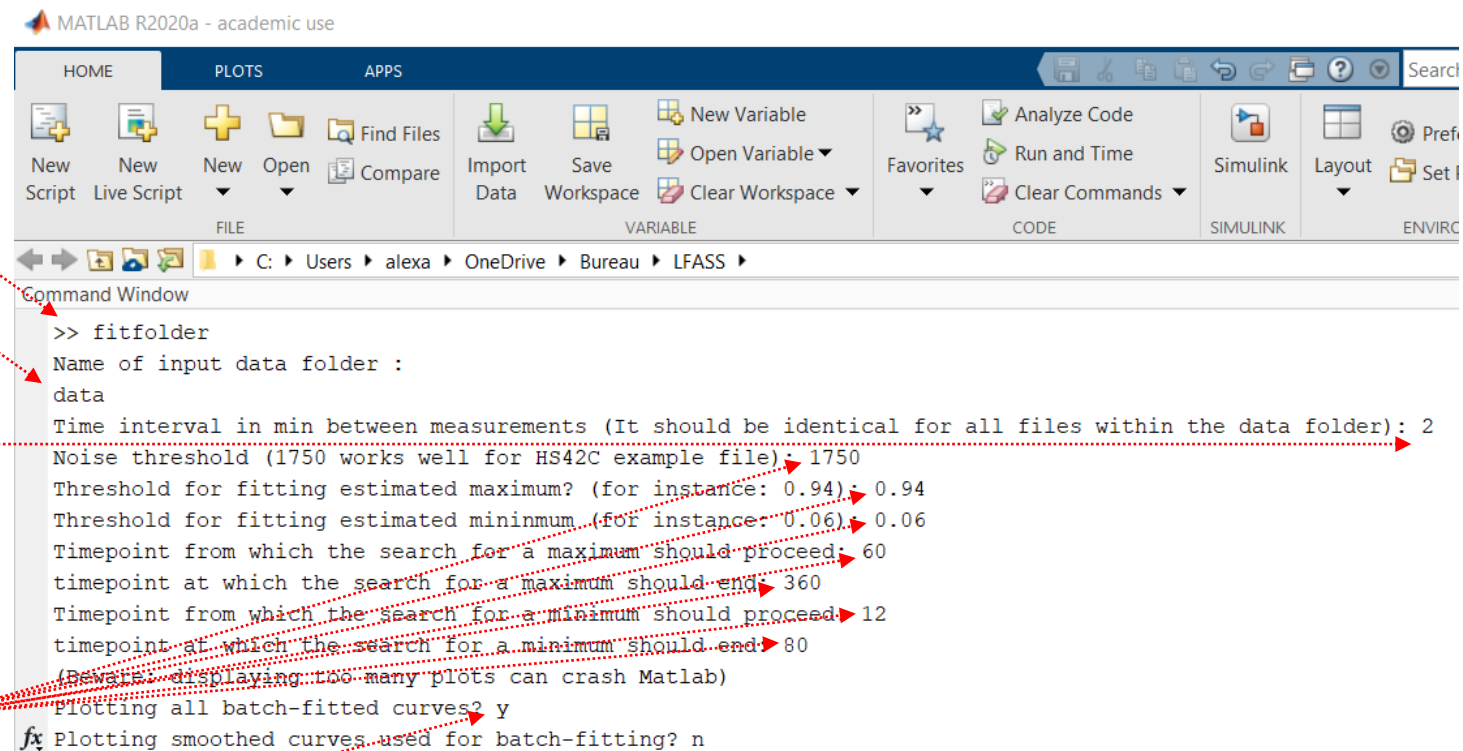
9. In the command window, type 'fitfolder', press 

10. Then enter the name of your data folder: 'data'

11. Enter the time interval between consecutive measurements of the same well (it should be an integer, here '2' for 2 min)

12. Enter other parameters pressing  each time.

13. Enter 'y' for YES to plot fitted curves



```
MATLAB R2020a - academic use

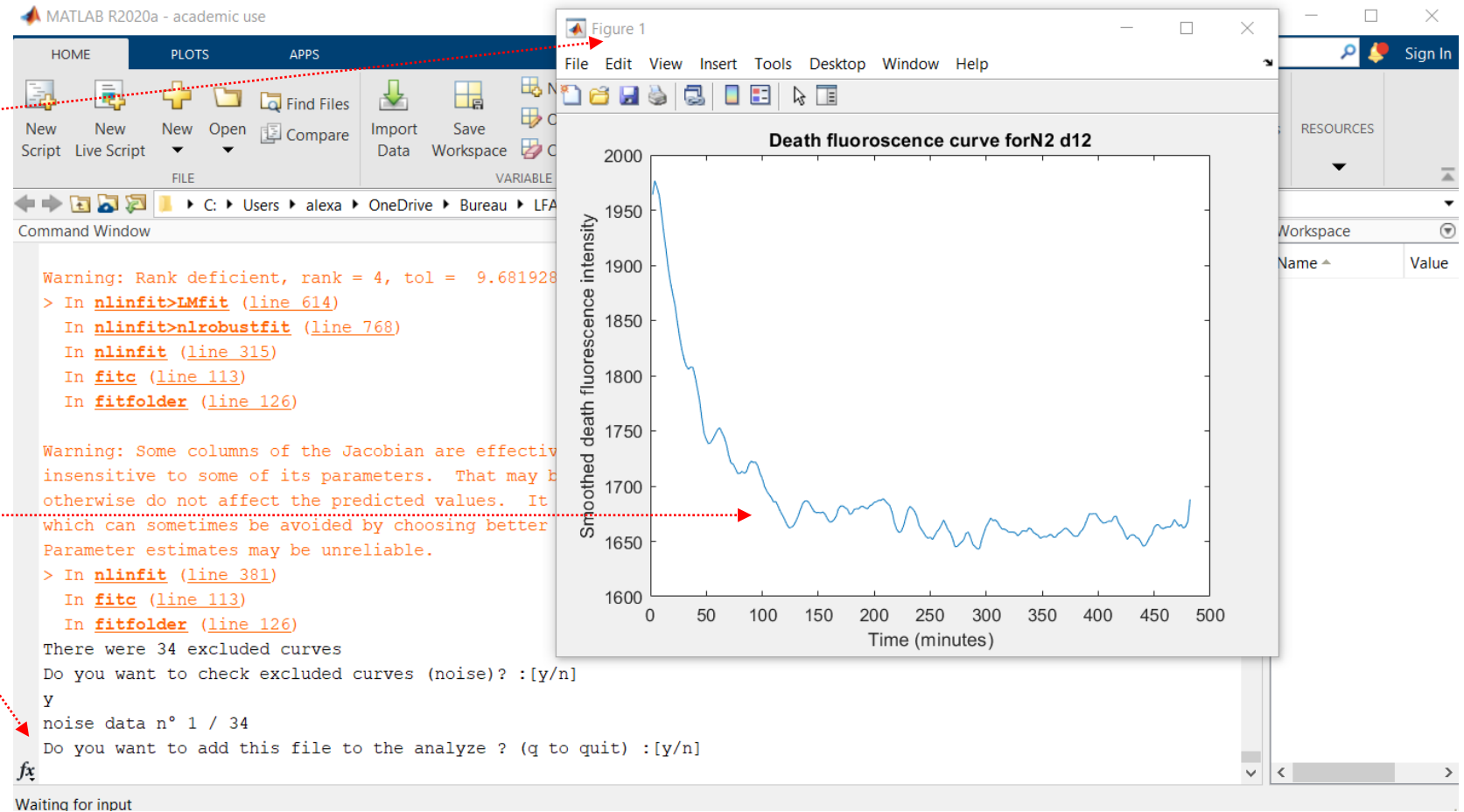
HOME PLOTS APPS
New Script New Live Script New Open Find Files Import Data Save Workspace New Variable Open Variable Clear Workspace Favorites Analyze Code Run and Time Clear Commands Simulink Layout Set I
FILE VARIABLE CODE SIMULINK ENVIRC

C:\Users\alexa\OneDrive\Bureau\LFASS
Command Window

>> fitfolder
Name of input data folder :
data
Time interval in min between measurements (It should be identical for all files within the data folder): 2
Noise threshold (1750 works well for HS42C example file): 1750
Threshold for fitting estimated maximum? (for instance: 0.94): 0.94
Threshold for fitting estimated minimum? (for instance: 0.06): 0.06
Timepoint from which the search for a maximum should proceed: 60
timepoint at which the search for a maximum should end: 360
Timepoint from which the search for a minimum should proceed: 12
timepoint at which the search for a minimum should end: 80
(Beware: displaying too many plots can crash Matlab)
Plotting all batch-fitted curves? y
Plotting smoothed curves used for batch-fitting? n
```

14. The routine will display excluded curves one by one querying whether it should be fitted

15. Enter 'y' to try to automatically refit the curve and 'n' if not (here the curve does not display any DF peak and is excluded from the analysis)



16. After all excluded curves have been checked or ignored, poorly-fitted curves are reviewed next.
17. Usually, these will be rechecked one by one and refitted using new time boundary parameters.
18. Type 'y' for YES, to enable review of ill-fitted curves one by one.

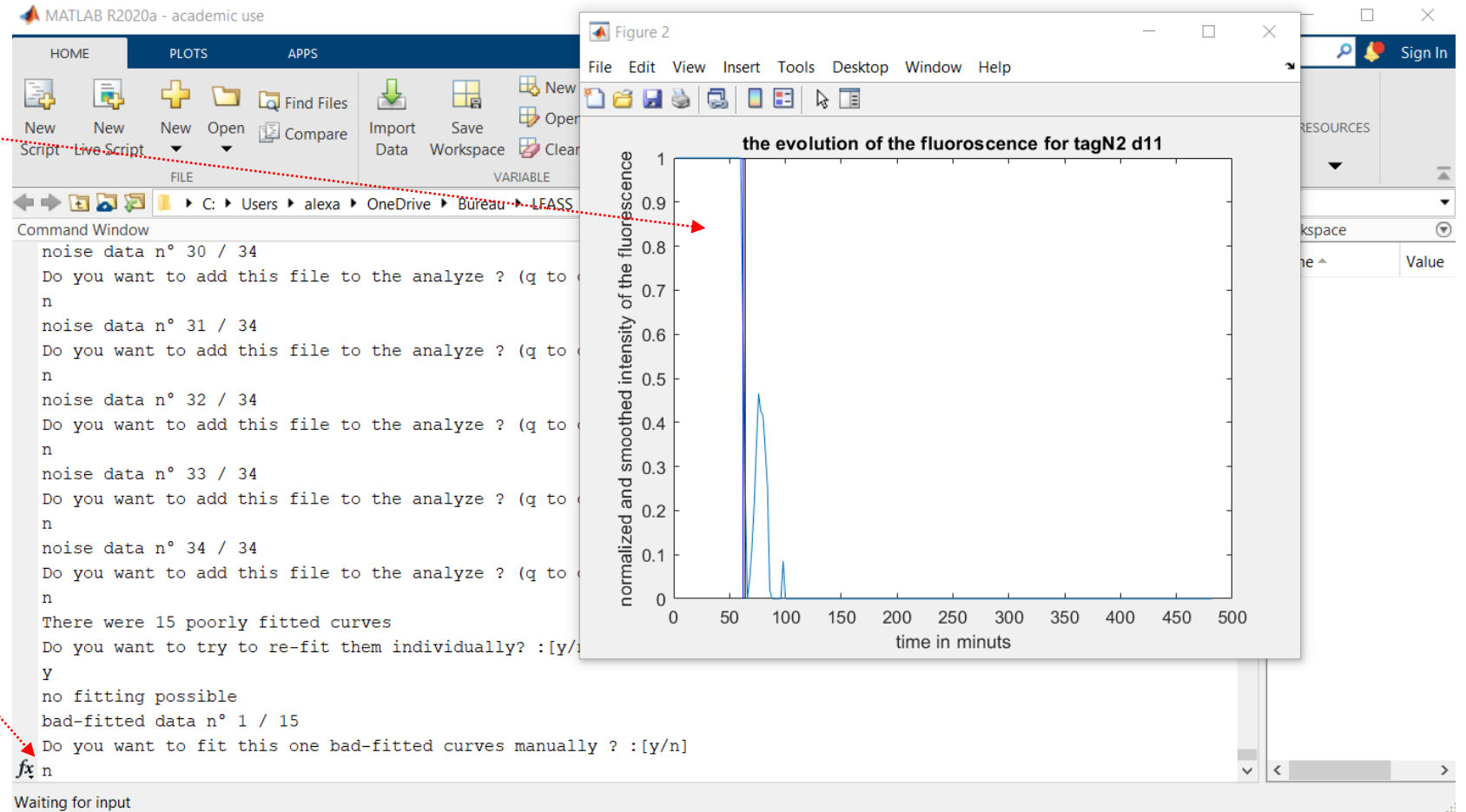
The screenshot shows the MATLAB R2020a - academic use interface. The Command Window displays a script that iterates through 34 noise data files, asking the user if they want to add each file to the analysis. The script has just finished processing file 34 and has identified 15 poorly fitted curves. A red arrow points from the text 'Type 'y' for YES, to enable review of ill-fitted curves one by one.' to the prompt 'Do you want to try to re-fit them individually? :[y/n]'. The Workspace panel on the right is empty.

```
n
noise data n° 29 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
noise data n° 30 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
noise data n° 31 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
noise data n° 32 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
noise data n° 33 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
noise data n° 34 / 34
Do you want to add this file to the analyze ? (q to quit) :[y/n]
n
There were 15 poorly fitted curves
Do you want to try to re-fit them individually? :[y/n]
```

Waiting for input

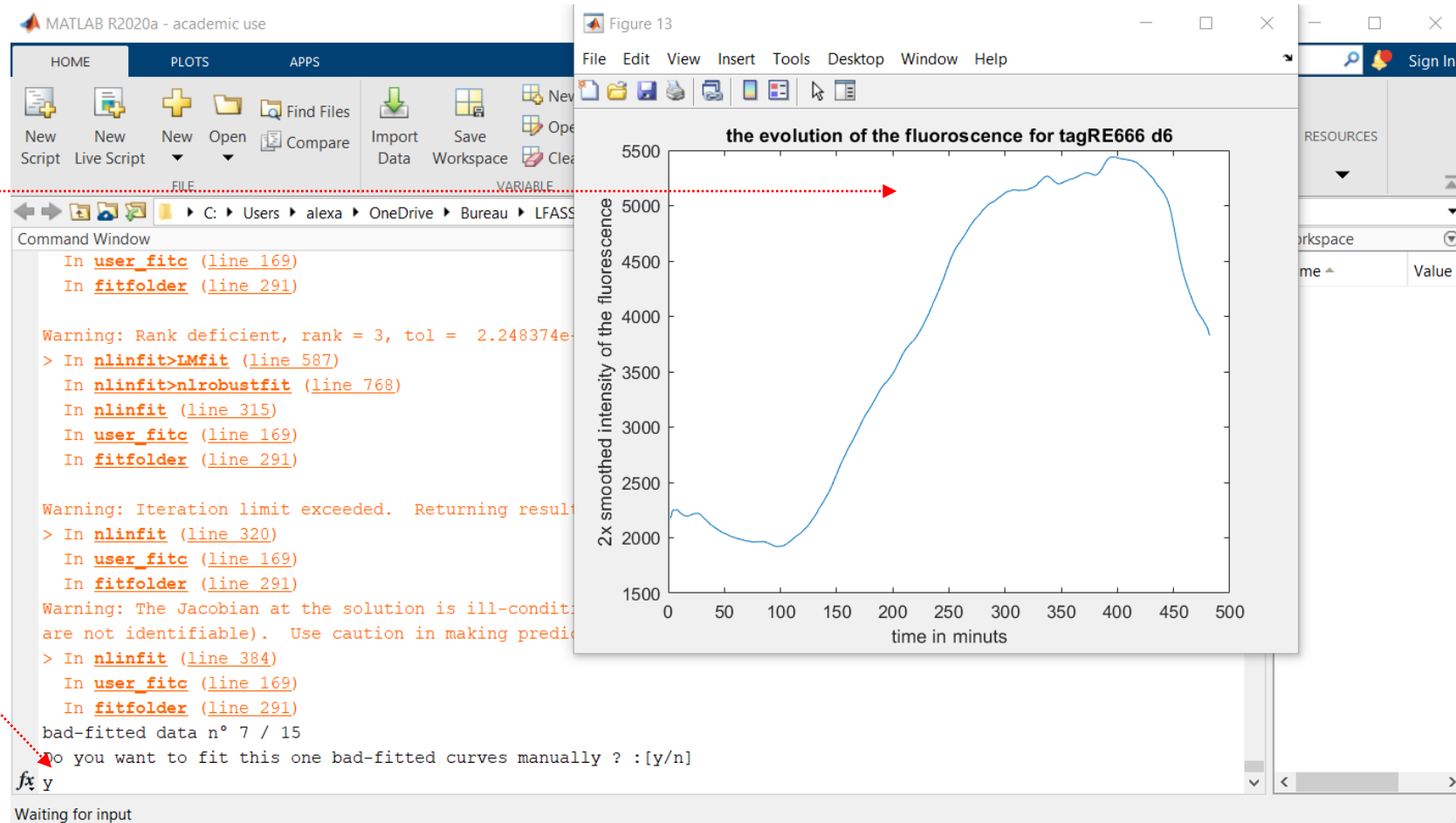
19. Here is an example of a failed fit where the curve does not show any clear DF peak.

20. Visual inspection here confirms that the curve does not contain useable data. Enter 'n' for NO to reject re-fitting.

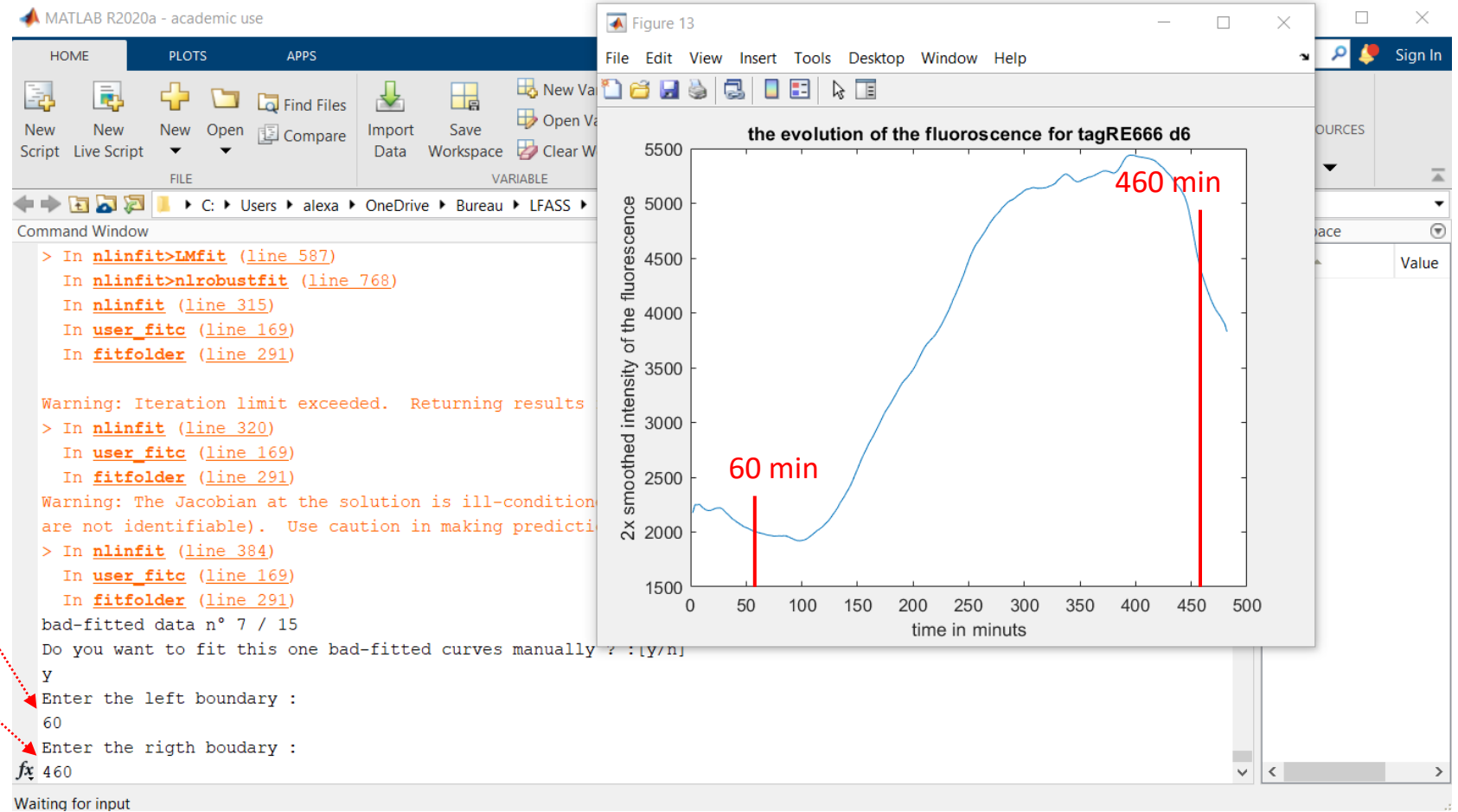


21. Here is an example of a failed fit where the curve shows a clear DF peak. The fit failed because the maximum (at ~400min) is found after the upper limit set earlier for the batch analysis (360 min, see step 12).

22. In this case the curve needs to be refitted. Enter 'y' for YES to re-fit.

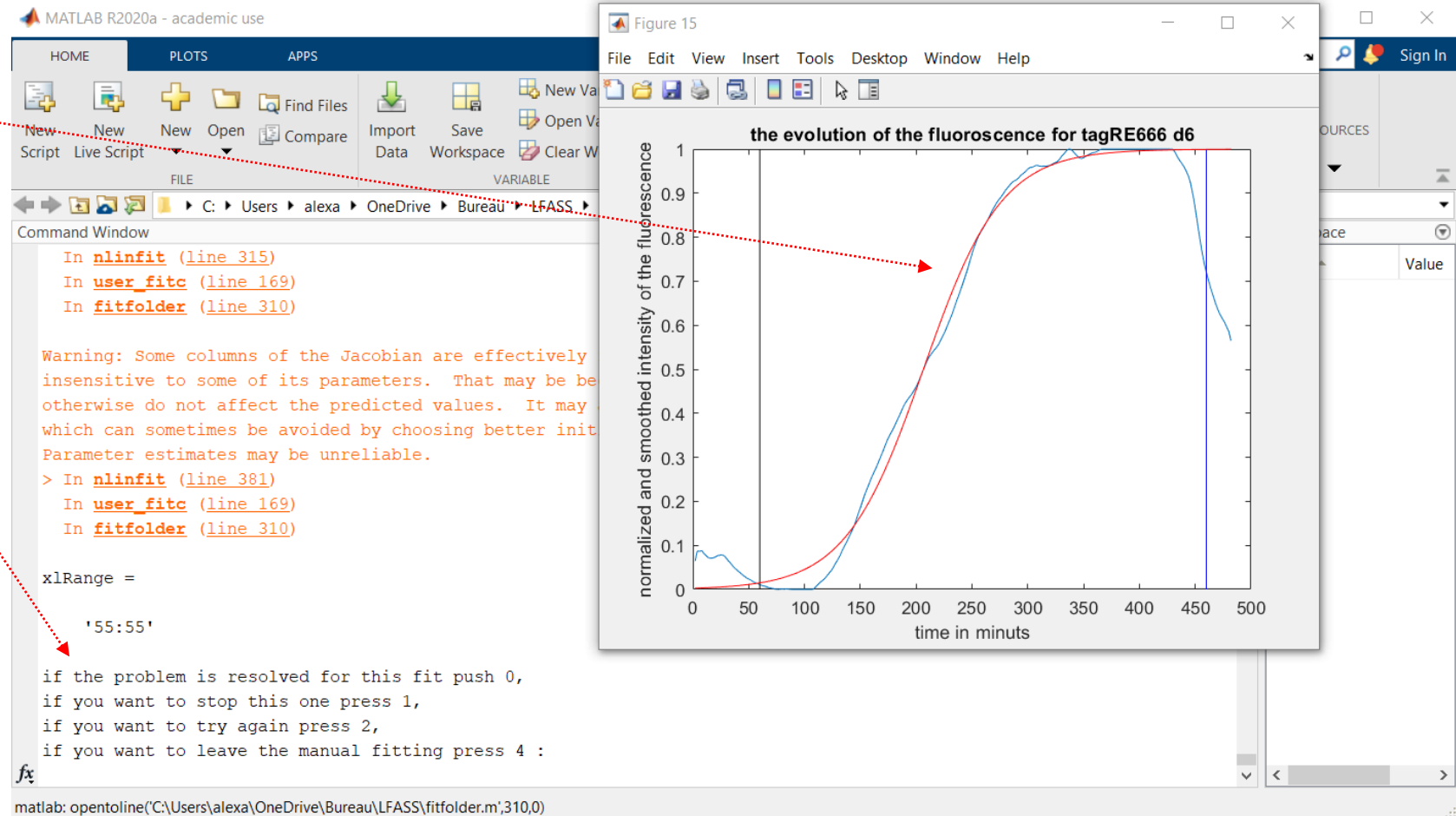


23. Enter new time boundaries that encompass the region of the curve where a sigmoid fit can be applied (for instance here between 60min and 460min)

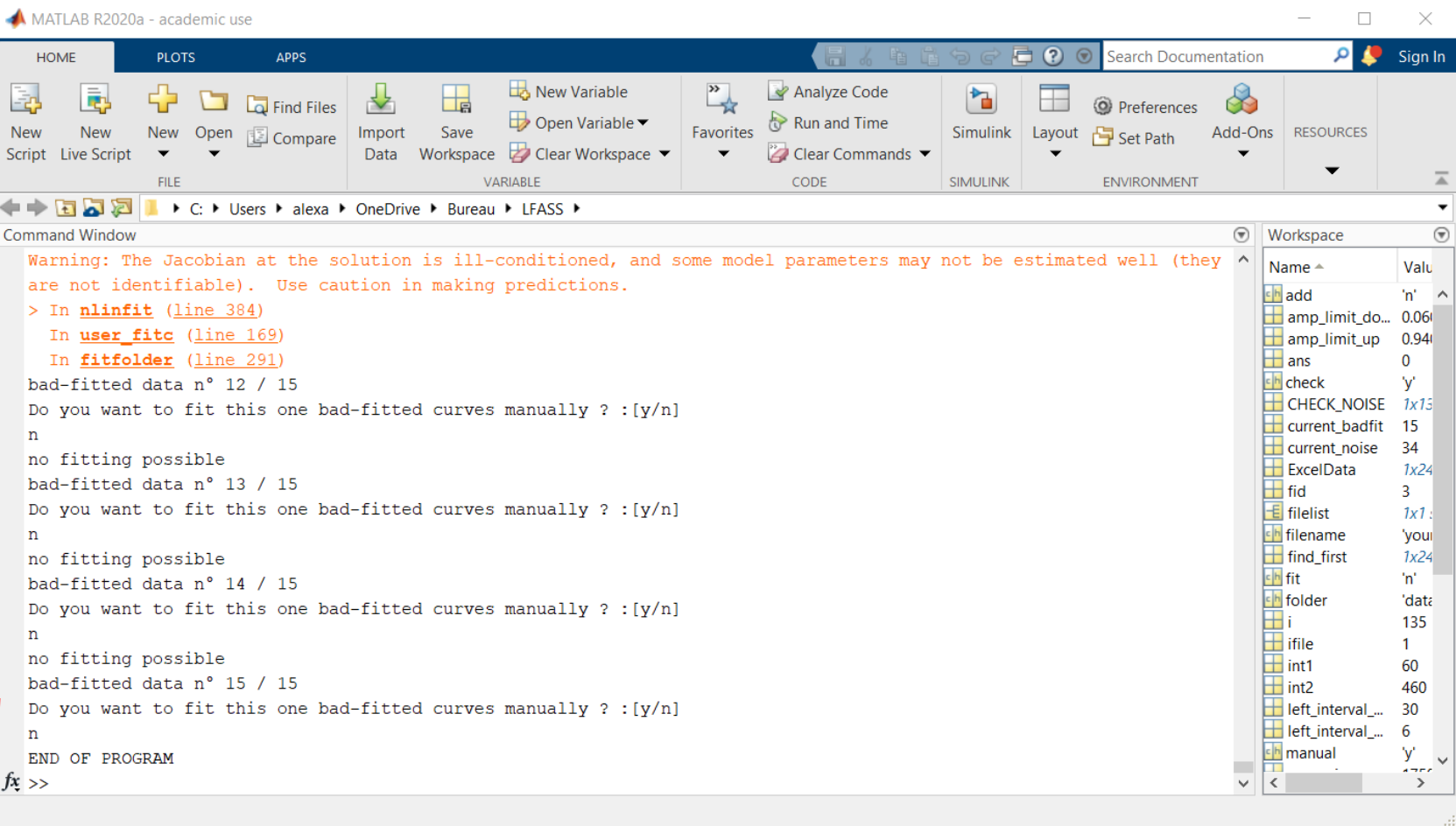


24. After fitting is reattempted, the result is displayed.

25. A choice is then given to accept the new fit (type '0'), or to reattempt it (type '2'). Typing '0' automatically moves to the next curve.



26. After refitting has been attempted or declined for all remaining curves, the program ends.



27. The result files are found in the 'results-folder'

LFASS > results_folder

Name	Status	Date modified	Type	Size
Batch analysis noise fitted	✓ R	13/04/2022 11:39	Text Document	4 KB
Batch analysis only	✓ R	13/04/2022 11:35	Text Document	4 KB
Refitted	✓ R	13/04/2022 11:46	Text Document	5 KB

28. Open the 'refitted.txt' file with Excel or equivalent (contains all the data)

AutoSave Off

File Home Insert Page Layout Formulas Data Review

Clipboard Font Alignment

Calibri 11

condition

	A	B	C	D	E	F
1	condition	Raw	Batch-fitted	Re-fitted		
2						
3						
4						
5	your-data-file.xlsx					
6	Raw data	0	0	0		
7	28800s	0	0	0		
8	41.9 Å°C	0	0	0		
9	N2 d1	88	8.66E+01	8.66E+01		
10	N2 d2	74	7.81E+01	7.81E+01		
11	N2 d4	128	1.27E+02	1.27E+02		
12	N2 d6	162	1.59E+02	1.59E+02		
13	N2 d7	148	1.48E+02	1.48E+02		
14	N2 d8	156	1.54E+02	1.54E+02		
15	N2 d9	106	1.10E+02	1.10E+02		
16	N2 d11	152	1	NaN		
17	N2 d12	1	1	1		
18	N2 d13	1	1	1		
19	N2 d14	1	1	1		
20	empty	1	1	1		
21	SJ17 d1	122	1.25E+02	1.25E+02		
22	SJ17 d2	116	1.18E+02	1.18E+02		

Refitted

29. Convert data to preferred number format (here .00, note re-fitted data line 60)

AutoSave On

File Home Insert Page Layout Formulas Data Review

Clipboard Font Alignment

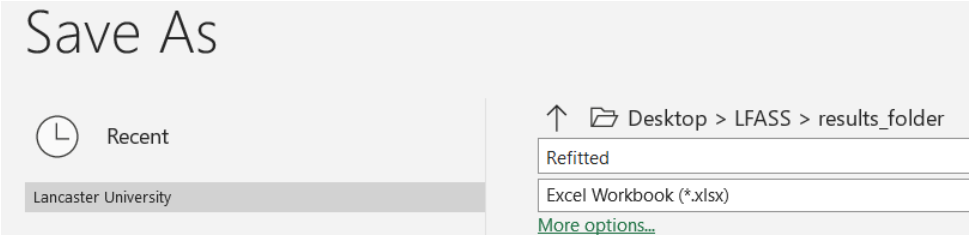
Calibri 11

RE666 d6

	A	B	C	D	E
52	SJ4005 d11	154.00	154.78	154.78	
53	SJ4005 d12	150.00	156.53	156.53	
54	SJ4005 d13	1.00	1.00	1.00	
55	SJ4005 d14	76.00	1.00	1.00	
56	empty	1.00	1.00	1.00	
57	RE666 d1	114.00	112.99	112.99	
58	RE666 d2	106.00	103.13	103.13	
59	RE666 d4	140.00	140.64	140.64	
60	RE666 d6	208.00	1.00	206.50	
61	RE666 d7	196.00	192.27	192.27	
62	RE666 d8	138.00	138.75	138.75	
63	RE666 d9	208.00	211.43	211.43	
64	RE666 d11	1.00	1.00	1.00	
65	RE666 d12	1.00	1.00	1.00	
66	RE666 d13	66.00	1.00	1.00	
67	RE666 d14	1.00	1.00	1.00	
68	RE666 d15	70.00	1.00	1.00	
69	VC893 d1	128.00	125.70	125.70	
70	VC893 d2	94.00	93.68	93.68	
71	VC893 d4	110.00	108.94	108.94	
72	VC893 d6	104.00	102.90	102.90	
73	VC893 d7	106.00	105.47	105.47	

Refitted

30. Save the updated file in a convenient format for further analyses such as data manipulation and statistics (here .xlsx)



The End