### M3-Machine learning on hyperspectral data - wheat trial



Nicolas Vuille-dit-Bille



### Agroscope: swiss federal institute for agricultural research

#### **Group:**

Cultivation Techniques and Varieties in Arable Farming

#### Team:

35 People

#### Domains of research:

- Agronomy
- Crop science

#### Main areas of work:

- Characterization of genotypes of field crops
- Improvement of management practices of field crops

#### **Crop species:**

- Winter cereals (wheat, barley, oat, ...)
- Maize
- Potato and Sugar beet
- Oil crops and grain legumes
- Minor crops (e.g. Quinoa, Amaranth)



# Variety trial context

Winter wheat varieties are tested on different experimental fields across Switzerland with different modality (low vs high inputs)

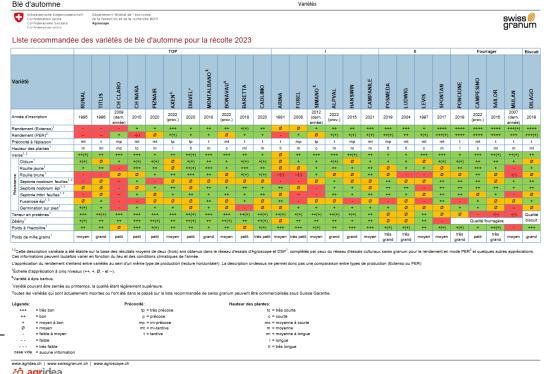
Each year, winter wheat varieties performance are reported and recommended to farmers according to a list

Challenge: not easy to estimate and understand accurately specific varieties response to specific environment linked to

abiotic and biotic stresses (uncontrolled factors on the field)



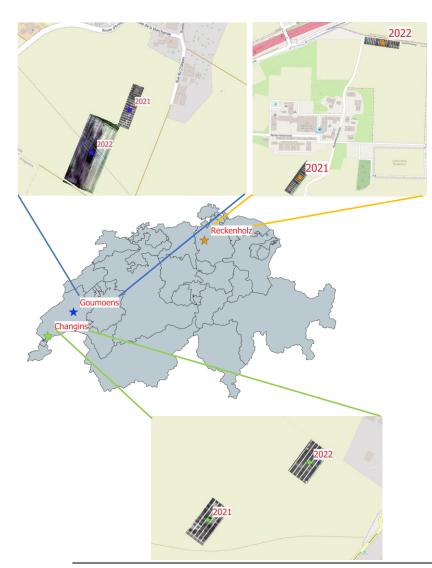


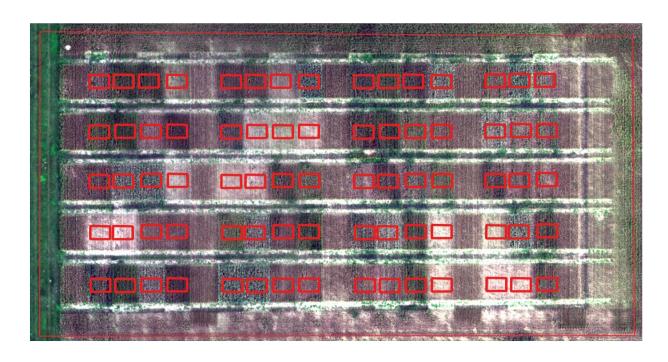


# Case study: winter wheat trial with 2 treatments over 2 years on 3 sites

- 5 winter wheat varieties
- 2 years: 2021 to 2022
- 3 sites: Changins, Goumoens and Reckenholz
- Case study context: study variety response to different N treatment
- Find variety that are performing well also under limited available N in order to reduce N fertilization (economic and environmental cost)
- 3 main treatments: none, reduced and conventional
- Measurement to estimate varieties performance:
- Grain yield
- Straw yield
- > Grain protein
- Other physiological parameters (harvest index, leaf area index, chlorophyll content, canopy cover...)

# Case study: field experimental design



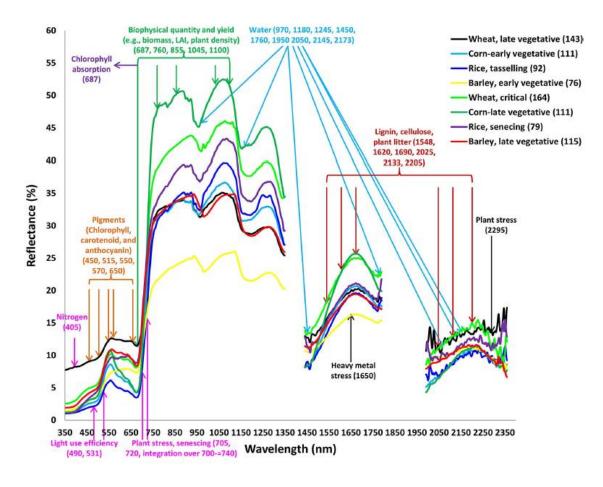


# **©** Case study: variety x N treatments

Treatment			Total N	
ID	Variety	N treatment	applied	N rate
1	CH Claro	N0	0 kgN/ha-1	0-0-0
2	CH Claro	N1	80 kgN/ha-1	20-40-20
3	CH Claro	N2	80 kgN/ha-1	20-60-0
4	CH Claro	N3	160 kgN/ha-1	40-80-40
5	CH Claro	N4	160 kgN/ha-1	40-120-0
6	CH Nara	N0	0 kgN/ha-1	0-0-0
7	CH Nara	N1	80 kgN/ha-1	20-40-20
8	CH Nara	N2	80 kgN/ha-1	20-60-0
9	CH Nara	N3	160 kgN/ha-1	40-80-40
10	CH Nara	N4	160 kgN/ha-1	40-120-0
11	CH Camedo	N0	0 kgN/ha-1	0-0-0
12	CH Camedo	N1	80 kgN/ha-1	20-40-20
13	CH Camedo	N2	80 kgN/ha-1	20-60-0
14	CH Camedo	N3	160 kgN/ha-1	40-80-40
15	CH Camedo	N4	160 kgN/ha-1	40-120-0
16	Montalbano	N0	0 kgN/ha-1	0-0-0
17	Montalbano	N1	80 kgN/ha-1	20-40-20
18	Montalbano	N2	80 kgN/ha-1	20-60-0
19	Montalbano	N3	160 kgN/ha-1	40-80-40
20	Montalbano	N4	160 kgN/ha-1	40-120-0
21	Runal	N0	0 kgN/ha-1	0-0-0
22	Runal	N1	80 kgN/ha-1	20-40-20
23	Runal	N2	80 kgN/ha-1	20-60-0
24	Runal	N3	160 kgN/ha-1	40-80-40
25	Runal	N4	160 kgN/ha-1	40-120-0

	Repetition 1					Repetition 2						Repetition 3						
	7	25	24	16	2	2	23	1	15		10	17	4	13		22	14	8
	N2	N5	N4	N0	N	12	N3	N0	N5		N5	N2	N4	N3		N2	N4	N3
	17	19	8	5	و	9	11	16	21		25	20	18	23		12	7	10
	N2	N4	N3	N5	N	14	N0	N0	N0		N5	N5	N3	N3		N2	N2	N5
	22	12	14	11	2	1	6	24	18		8	4	9	17		5	2	3
	N2	N2	N4	N0	N	10	N0	N4	N3		N3	N4	N4	N2		N5	N2	N3
	1	6	23	3	1	8	13	5	19		9	12	20	11		16	15	24
	N0	N0	N3	N3	N	13	N3	N5	N4		N4	N2	N5	N0		N0	N5	N4
	10	20	13	4	1	5	14	2	3		22	7	19	21		6	1	25
Г	N5	N5	N3	N4	N	15	N4	N2	N3		N2	N2	N4	N0	1	N0	N0	N5

# Hyperspectral data: theory



Thenkabail, P. S., Mariotto, I., Gumma, M. K., Middleton, E. M., Landis, D. R., & Huemmrich, K. F. (2013). Selection of hyperspectral narrowbands (HNBs) and composition of hyperspectral twoband vegetation indices (HVIs) for biophysical characterization and discrimination of crop types using field reflectance and Hyperion/EO-1 data. IEEE Journal of Selected Topics in Applied Earth Observations and Remote Sensing, 6(2), 427-439. https://doi.org/10.1109/JSTARS.2013.2252601



### Hyperspectral data collection

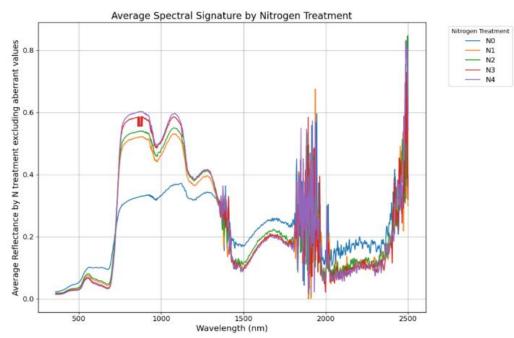
	ID	CropStage	rflt_359	rflt_360	rflt_361	rflt_362	rflt_363	rflt_364	rflt_365	rflt_366	
450	1	Heading	0.018496	0.018435	0.018400	0.018405	0.018403	0.018397	0.018387	0.018440	
451	2	Heading	0.020588	0.020687	0.020785	0.020865	0.020946	0.021021	0.021073	0.021132	
452	3	Heading	0.011134	0.011124	0.011104	0.011091	0.011060	0.011027	0.011021	0.011047	
453	4	Heading	0.014384	0.014365	0.014328	0.014269	0.014220	0.014181	0.014157	0.014164	
454	5	Heading	0.031535	0.031565	0.031607	0.031671	0.031738	0.031801	0.031855	0.031862	

Time series data corresponding to key crop growth stage

> 2 years: 2021-2022

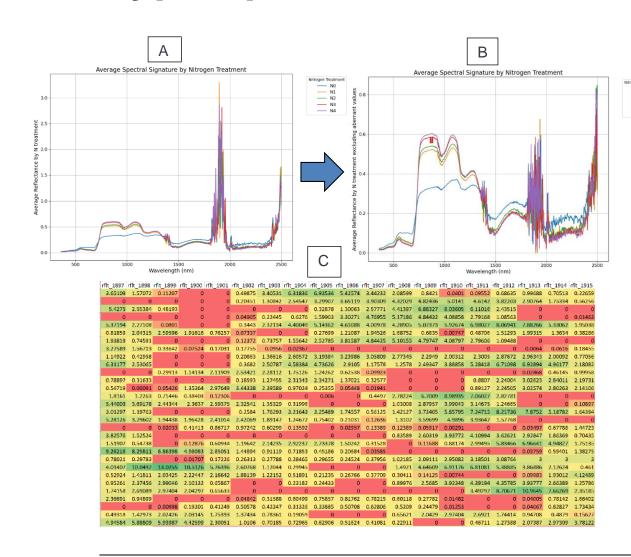
> 3 sites: Changins, Goumoens and Reckenholz





### 0

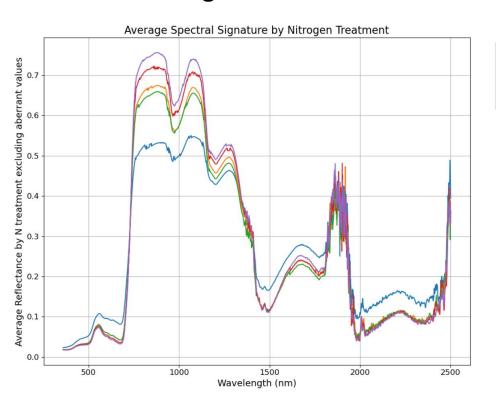
### Hyperspectral data cleaning



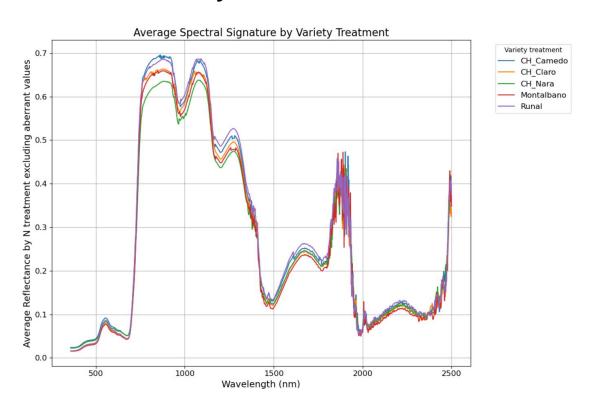
- > Remove bands with aberrant values: <0 or >1
- > Remove bands with 0 value

# Average of spectral signature by treatments at heading

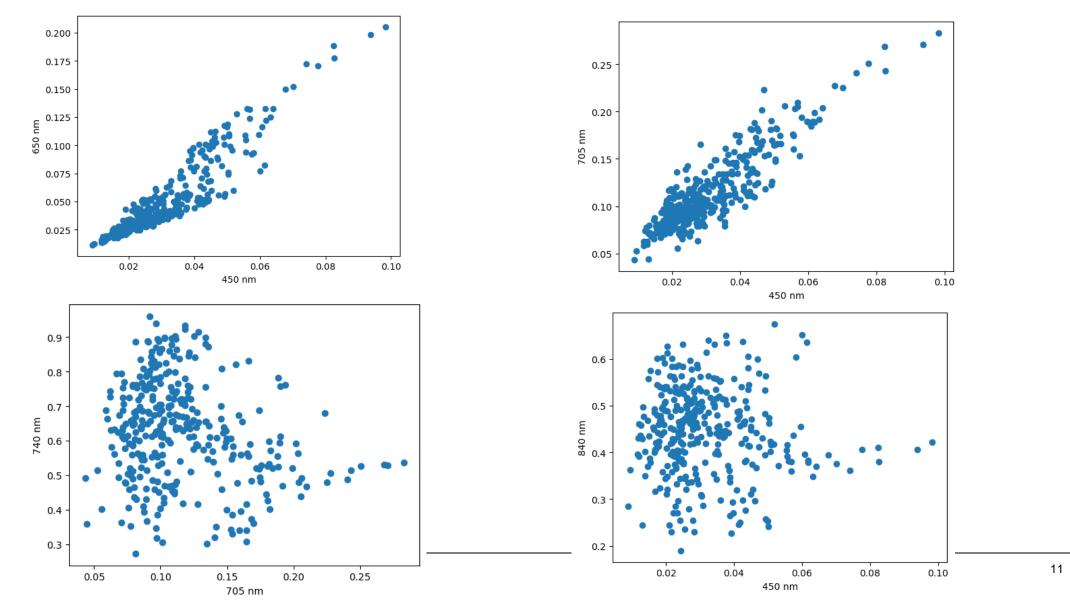
#### Nitrogen treatment



#### Variety treatment

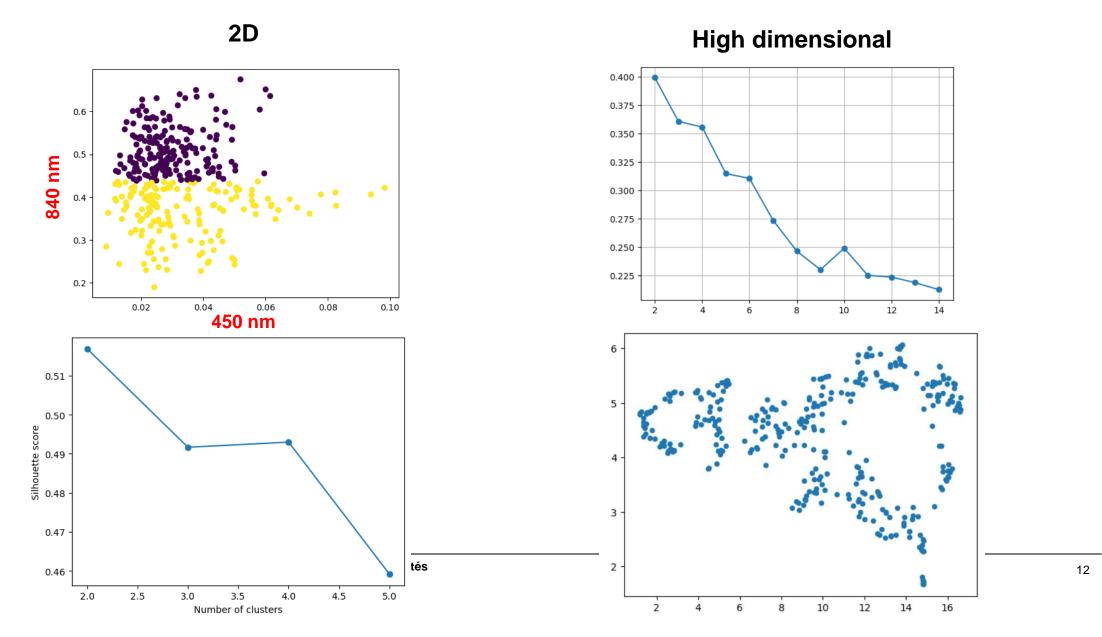


# **U** Hyperspectral: highly intercorrelated

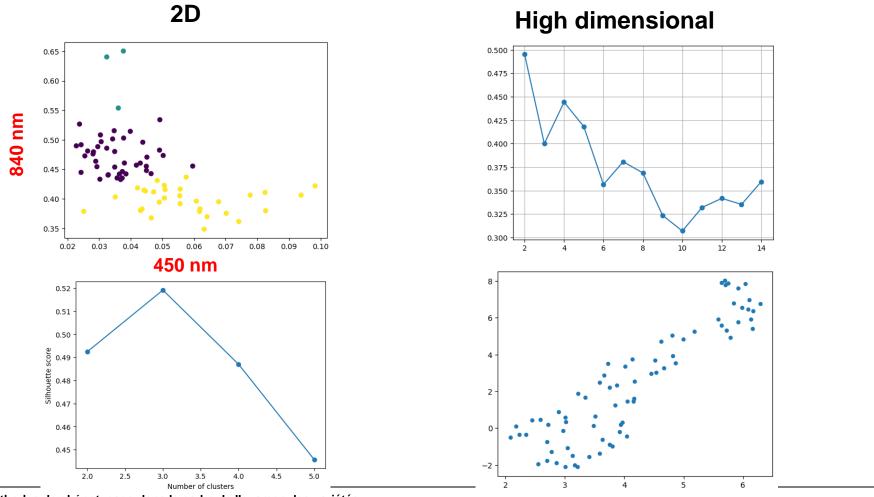


### V

# Data exploration: clustering (K-means) and umap

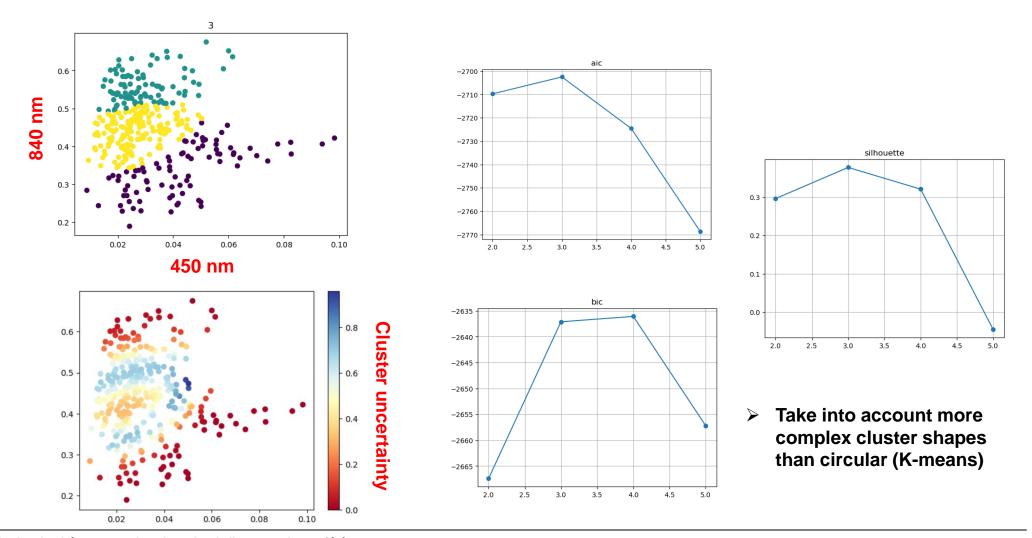


# Data exploration: clustering (K-means) and umap – Focusing on Changins in 2022



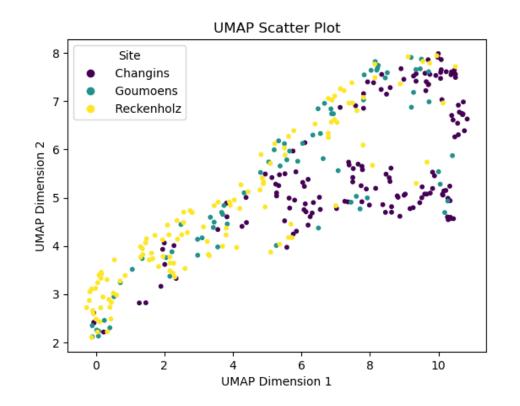


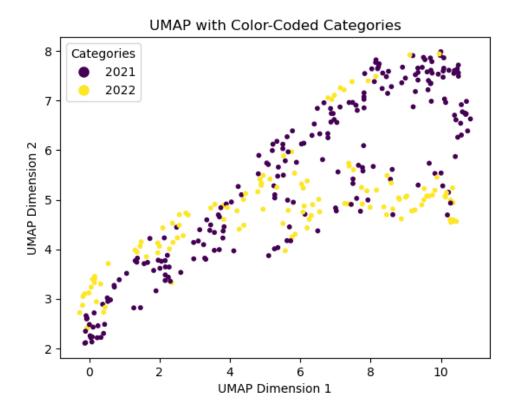
# Data exploration: Gaussian mixtures (soft clustering)





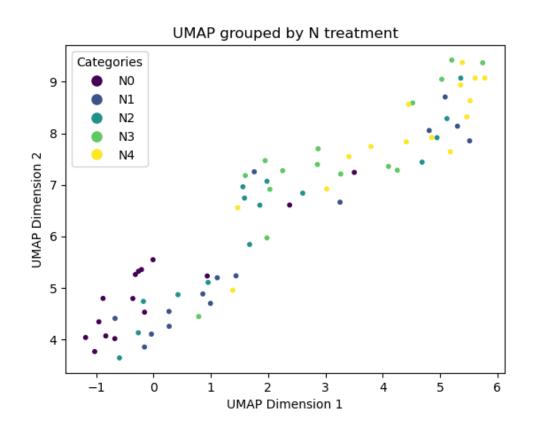
# Data exploration: umap

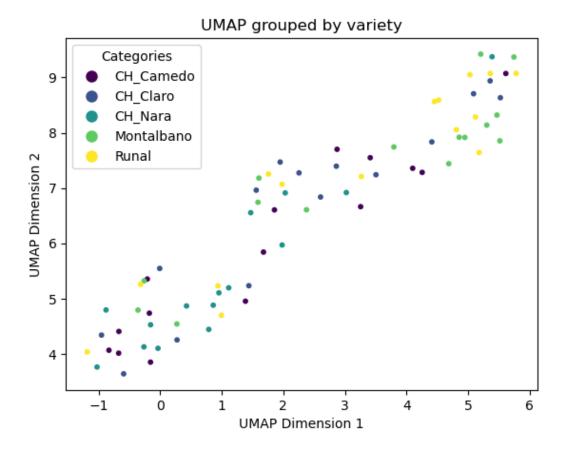




### **O**

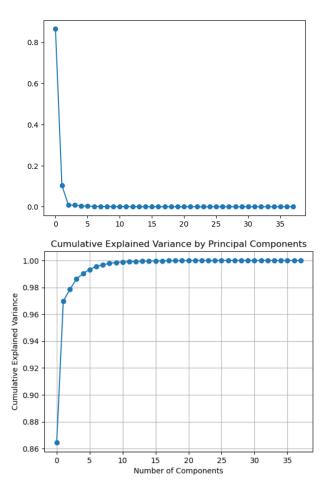
# Data exploration: umap-focus on Changins 2022







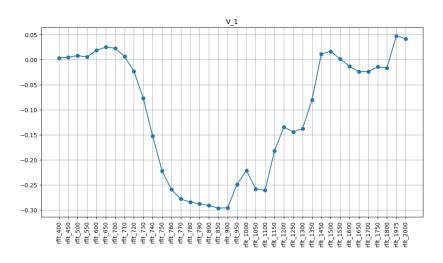
# **Data exploration: PCA**

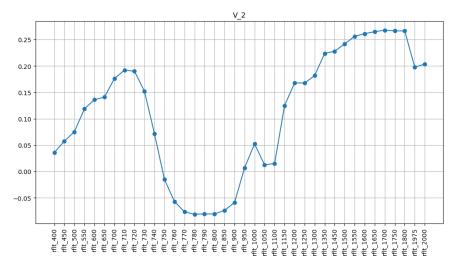


Most of the variance is explained by the first principal components

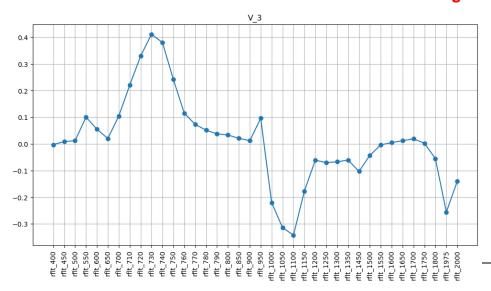
	V_1	V_2	V_3	V_4	V_5	V_6	V_7	V_8	V_9	V_10	 V_29	V_30	V_31	V_32	
rflt_400	0.002937	0.035984	-0.002985	0.036265	-0.066545	-0.077143	0.047143	0.018090	0.027047	-0.030372	 -0.314811	0.013153	0.370203	-0.570470	-
rflt_450	0.004546	0.057737	0.008797	0.048449	-0.083053	-0.093928	0.058513	0.031172	0.033828	-0.038866	 -0.097061	0.031067	-0.051995	0.439703	
rflt_500	0.007968	0.075280	0.011633	0.057094	-0.102647	-0.111227	0.070736	0.038209	0.045630	-0.059384	 0.001776	0.045085	-0.137613	0.450820	
rflt_550	0.004938	0.118608	0.100272	0.041700	-0.076588	-0.132578	0.133371	0.025159	0.008326	-0.070819	 0.464148	-0.161390	-0.025780	-0.243287	-
rflt_600	0.018468	0.136195	0.055064	0.063748	-0.126743	-0.139727	0.104721	0.041003	0.076547	-0.104400	 0.177287	-0.002736	-0.130536	-0.221454	-
rflt_650	0.024707	0.141009	0.020273	0.078288	-0.151596	-0.132552	0.071822	0.055425	0.113306	-0.113475	 -0.030904	0.120243	-0.309854	-0.225976	
rflt_700	0.022719	0.176140	0.104292	0.057160	-0.127722	-0.154214	0.136993	0.031696	0.086213	-0.128917	 -0.135049	-0.047044	0.202034	0.128728	-
rflt_710	0.005987	0.192111	0.219704	0.011086	-0.058324	-0.144916	0.194052	-0.000885	0.026911	-0.131047	 -0.078937	-0.051935	0.400239	0.239990	-
rflt_720	-0.023342	0.190195	0.329054	-0.035184	0.022756	-0.115419	0.246817	-0.045449	-0.020716	-0.097410	 -0.127544	-0.031272	-0.026472	0.001404	
rflt_730	-0.077068	0.152240	0.411113	-0.068129	0.120301	-0.045753	0.256434	-0.071563	-0.090646	-0.021463	 -0.054480	0.214311	-0.510202	-0.139891	-
rflt_740	-0.152834	0.071806	0.380125	-0.038900	0.173887	0.054169	0.161227	-0.040682	-0.175539	0.090713	 0.178868	-0.147663	0.331254	0.042661	-
rflt_750	-0.222108	-0.014992	0.241446	0.043583	0.144238	0.120612	-0.003116	0.014278	-0.249012	0.255482	 -0.165143	0.008243	0.025910	0.019577	
rflt_760	-0.259550	-0.056748	0.115213	0.092566	0.044302	0.060705	-0.063564	0.019648	-0.047796	0.043965	 0.085799	0.072182	0.095962	0.029375	
rflt_770	-0.278402	-0.076261	0.073083	0.133530	0.008369	0.075799	-0.126264	0.056414	-0.127857	0.132030	 0.083548	0.064112	-0.139257	0.047678	-
rflt_780	-0.284698	-0.080844	0.051317	0.147931	-0.025486	0.047185	-0.127509	0.068652	-0.105174	0.070686	 0.183179	0.033072	0.105926	-0.091678	
rflt_790	-0.288159	-0.080257	0.037642	0.151115	-0.061858	0.003719	-0.104245	0.053524	-0.021094	-0.036496	 -0.215291	-0.330882	-0.070489	-0.058744	
rflt_800	-0.291212	-0.080241	0.033173	0.157454	-0.080462	-0.012503	-0.093401	0.051798	-0.008328	-0.066501	 -0.274390	-0.159398	-0.253548	0.038784	-
rflt_850	-0.296626	-0.073656	0.020933	0.160679	-0.134902	-0.071902	-0.069440	0.053835	0.047964	-0.159894	 0.080215	0.707552	0.197408	0.016602	
rflt_900	-0.296011	-0.058551	0.011742	0.145246	-0.168055	-0.097280	-0.043212	-0.042513	0.242654	-0.185614	 0.148816	-0.454504	-0.026414	0.022098	
rflt_950	-0.249193	0.007015	0.095887	0.063978	-0.050155	0.033271	-0.047558	-0.215876	0.580823	0.068516	 -0.024967	0.096911	0.030991	-0.013949	
rflt_1000	-0.221344	0.052433	-0.220139	-0.169310	0.070945	-0.052127	0.170324	0.011850	-0.180992	-0.034090	 -0.045098	0.002954	0.015247	-0.014242	
rflt_1050	-0.258284	0.012576	-0.313951	-0.141051	-0.033743	-0.144897	0.224923	0.084717	-0.242277	-0.161996	 0.012214	0.006920	-0.014762	0.018567	
rflt_1100	-0.261066	0.015344	-0.341905	-0.131394	-0.048759	-0.162334	0.248113	0.035208	-0.147742	-0.133742	 -0.004369	0.022071	0.022281	-0.015644	-
rflt_1150	-0.182186	0.125109	-0.177318	-0.205285	0.048684	0.042876	0.155912	-0.196696	0.381576	0.250415	 0.039289	0.045725	0.026331	0.011381	
rflt_1200	-0.134697	0.167963	-0.061158	-0.194213	0.145048	0.106900	0.001842	-0.009889	0.045947	0.031876	 -0.164195	0.045232	-0.026473	-0.007882	
rflt_1250	-0.144183	0.167683	-0.070284	-0.202348	0.144352	0.106196	0.008684	0.024206	-0.016463	-0.010005	 0.433927	-0.070000	-0.027036	0.039075	-
rflt_1300	-0.137737	0.181770	-0.067180	-0.201547	0.131538	0.103304	0.011670	-0.011545	0.046018	0.005243	 -0.329916	-0.080701	-0.022178	-0.038984	
rflt_1350	-0.081059	0.223784	-0.060618	-0.151056	0.067630	0.086480	-0.000640	-0.083112	0.208114	0.205121	 0.029125	0.006407	-0.002334	0.015347	-
rflt_1450	0.011202	0.227878	-0.103072	0.166558	-0.268382	-0.401319	0.014654	0.149950	-0.105201	0.733861	 -0.001113	-0.017803	-0.011077	-0.002601	
rflt_1500	0.016259	0.241944	-0.042922	0.086942	-0.118142	-0.025608	-0.123851	0.219955	0.020149	-0.118426	 -0.014608	-0.007850	0.035438	0.014579	-
rflt_1550	0.001391	0.256196	-0.003615	0.008483	-0.061399	0.037940	-0.191749	0.202485	-0.008351	-0.131753	 -0.052260	0.047501	-0.000355	-0.024791	-
rflt_1600	-0.013472	0.261232	0.004638	-0.027502	0.010186	0.088423	-0.193448	0.185481	-0.010470	-0.086758	 -0.029999	-0.034136	0.015457	-0.008421	-
rflt 1650	-0.024138	0.265059	0.012019	-0.051561	0.037006	0.103989	-0.215153	0.144908	-0.025571	-0.065104	 0.013342	0.004593	0.012563	0.004921	

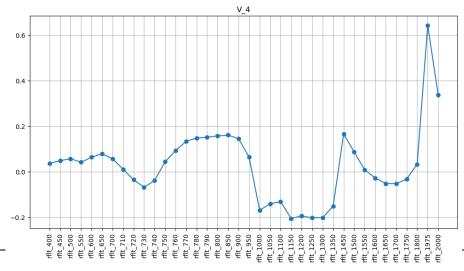
# **Data exploration: PCA**





#### 38 features at the beginning → 17 features selected





#### V1:

- > 900 nm
- ➤ 850 nm
- ➤ 800 nm
- > 790 nm
- > 780 nm
- > 770 nm

#### V2:

- > 700 nm
- > 710 nm
- > 720 nm
- > 1800 nm
- > 1550 nm

#### V3:

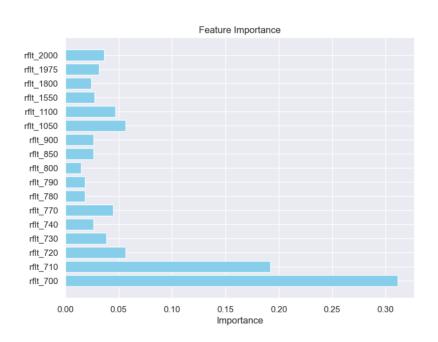
- > 730 nm
- > 740 nm
- > 1050 nm
- > 1100 nm

#### V4:

- > 1975 nm
- > 2000 nm

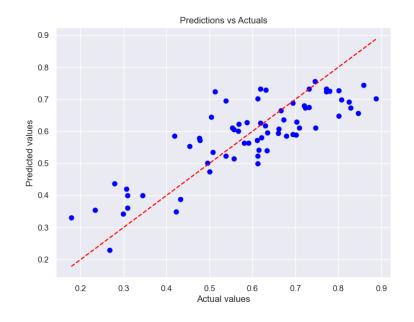
#### O

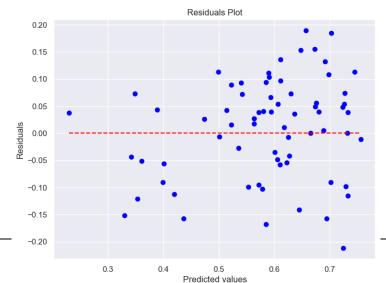
### Random forest model with selected features



Training R-squared: 0.955

Test R-squared: 0.685



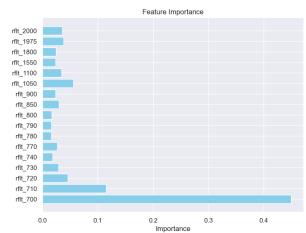




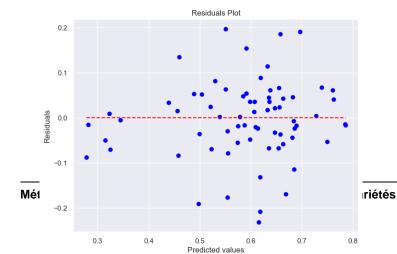
#### Random forest model with selected features: improvement tests

- Splitting train and test sets according to years or sites
- > Reducing the tree depth (max\_depth) and increasing the number of trees (n\_estimators)

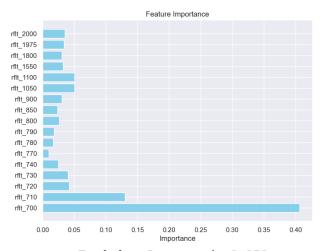




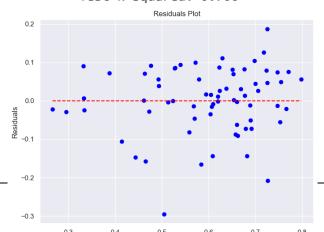
Training R-squared: 0.954 Test R-squared: 0.676



#### Years



Training R-squared: 0.950 Test R-squared: 0.706



Predicted values

### Conclusion

- Field data can be noisy:
- > Hyperspectral data is highly sensitive to weather conditions
- Promising results in data exploration (PCA):
- ➤ Highlighted the importance of red-edge bands between 700 to 800 nm to be able to characterize winter wheat performance
- Promising results in random forest:
- ➤ Highlighted the 700-710 nm part of the spectrum to explain grain yield differences
- ➤ It was expected because in theory it is linked to Nitrogen (N) chlorophyll content which is in this context (different levels of N treatments) an important indicator of grain yield
- Low performance in the test set compared to the training set:
- > Overfitting?
- Other agronomic parameter could be analysed to link to hyperspectral data
- Straw yield (positively correlated with grain yield)
- ➤ Harvest index (indicates the ratio of grain on total plant weight (grain + straw)
- Protein in grain (negatively correlated with grain yield)
- > Plant height (positively correlated with grain and straw yield; lodging effect)
- Disease (can explain unexpected low yield)

























### Thank you for your attention

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