Automatic classification of metal alloys from their LIBS spectra and its robustness against spectrometer decalibration

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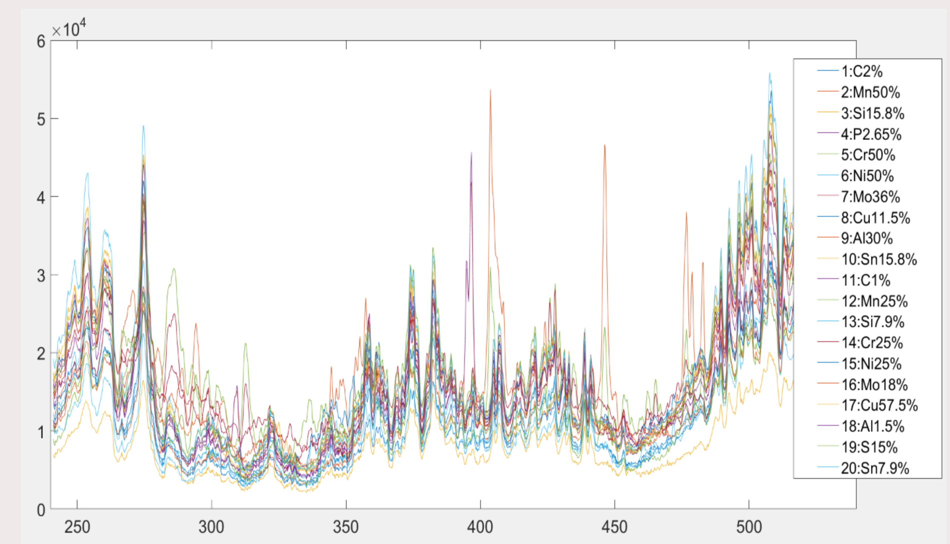
1 The problem

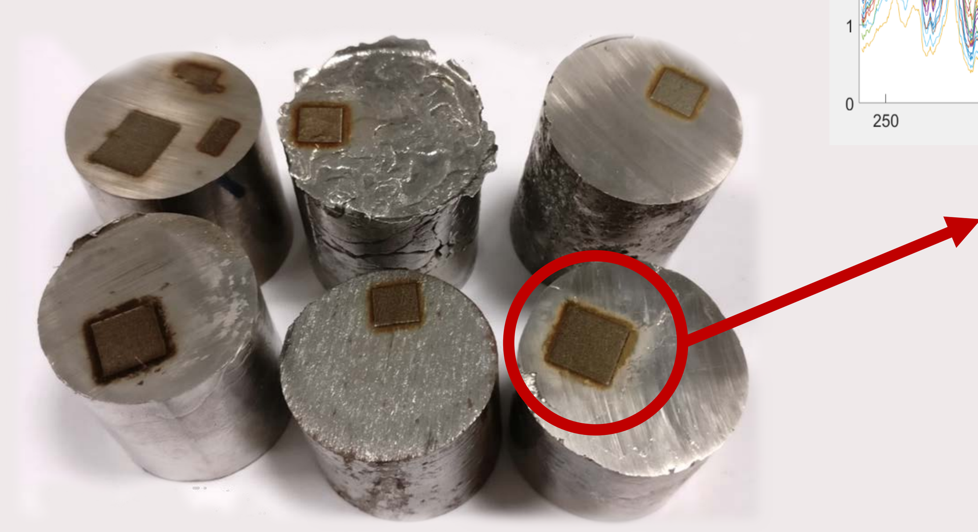
In **metal scrap sorting industry**, an online identification system would enable automatic sorting based on value, recycling requirements, presence of hazardous materials … LIBS has probed a suitable technique. However, simultaneous identification of some elements (Phosphor, Sulfur…) is not easy and instrumentation cost is an issue. If **low-cost spectrometers** are used, **long-term decalibration** due to thermal drift, shocks or ageing could drastically impact the classification performance.

2 Our proposal

In this work, we propose the use of **deep-learning algorithms** for automatic classification using raw LIBS spectra in a wide spectral window with low resolution, avoiding the preprocessing or the peaks/elements identification step. This approach enables the use of low cost spectrometers and simplify the processing software in operation once the deep network has been trained. However, **it could be very sensitive to the long-term decalibration of the spectrometer.**

We have measured 20 ingots of Iron alloy made in a levitation melting induction furnace, each one with different proportions of a single element commonly found in steel alloys: C, Mn, Si, P, Cr, Ni, Mo, Cu, Al, S & Sn.



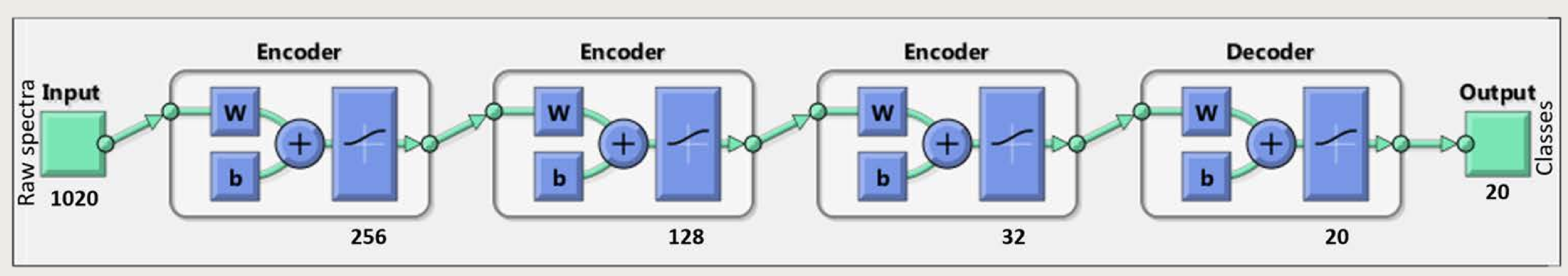


At least 10,000 LIBS spectra from each sample (1064nm Nd:YAG laser, 16ns pulse, 240-518nm spectral window, 0.5µs delay, 20 µs integration time) have been obtained.

3 Classification

A deep network of stacked autoenconders has been implemented in Matlab®, with 1020 neurons in the input layer, and 3 internal layers of 256, 128 and 32 neurons. A soft-max classifier with 20 outputs gives the predicted class.

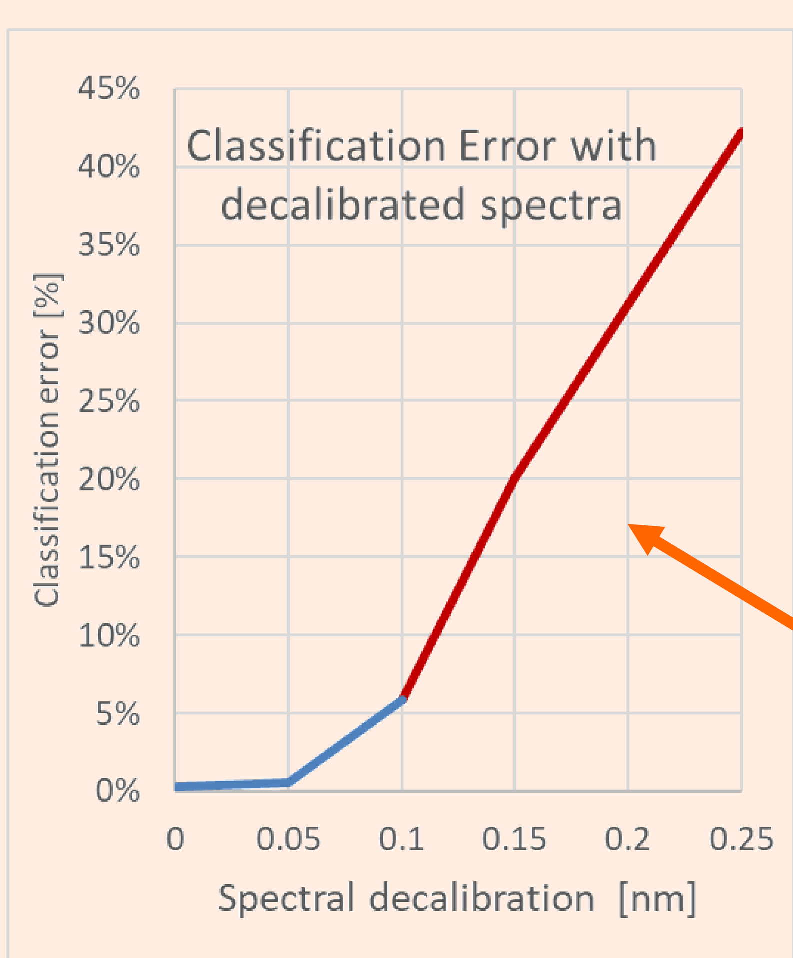
The network has been trained with 5,000 raw spectra from each ingot, preserving the intrinsic shot-to-shot intensity variations. The classification performance with **new spectra not used for training** shows a 0.3% classification error.



	C 2%	Mn 50%	Si 15.8%	P 2.65%	Cr 50%	Ni 50%	Mo 26%	Cu 11.5%	Al 30%	Sn 15.8%	C 1%	Mn 25%	Si 7.9%	Cr 25%	Ni 25%	Mo 18%	Cu 57.5%	Al 15%	S 15%	Sn 7.9%
1 C 2%	99.19%																			
2 Mn 50%		100.00%										0.05%								
3 Si 15.8%			96.98%																	
4 P 2.65%				99.98%							0.05%								0.07%	
5 Cr 50%					100.00%															
6 Ni 50%						99.98%														
7 Mo 36%							100.00%													
8 Cu 11.5%			0.01%					100.00%												
9 Al 30%									99.99%		0.02%									
10 Sn 15.8%										99.78%										1.46%
11 11: C 1%	0.81%		0.82%								99.87%									
12 Mn 25%			1.50%								0.05%	99.95%							0.06%	
13 Si 7.9%													99.99%						0.03%	
14 Cr 25%														100.00%						
15 Ni 25%															100.00%					
16 Mo 18%			0.05%													99.96%				
17 Cu 57.5%			0.05%							0.05%						0.01%	99.97%			0.05%
18 Al 15%																	0.01%	99.99%		
19 S 15%			0.03%																99.83%	
20 Sn 7.9%										0.17%										98.48%

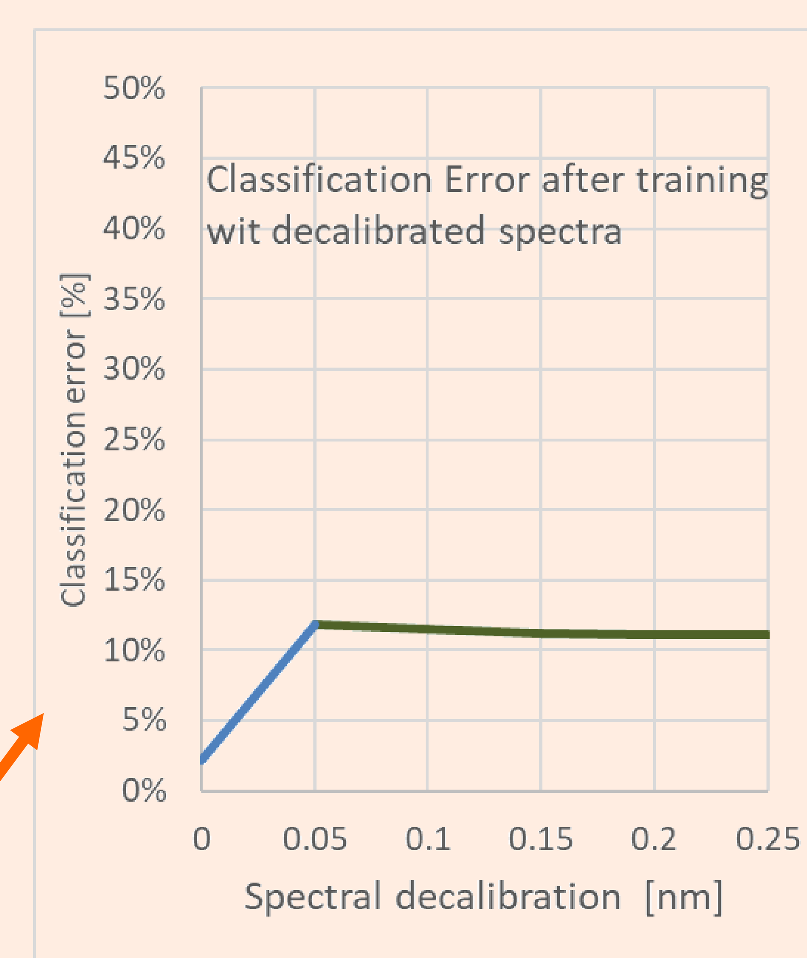
Error: 0.3%

4 Decalibration



However, the **expected long-term wavelength decalibration** of the spectrometer should affect the classification performance (+/- 0.25nm deviation for a 10ºC temperature change has been reported). The measured spectra have been artificially decalibrated and the robustness of classification has been obtained.

But … training the network with randomly and **purposely decalibrated** data reduce the classification error in the long term.



5 Conclusions

Deep ANN networks provide an almost black-box classification tool from raw LIBS spectra, but it is very sensitive to the small wavelength decalibration that is expected from long-term operation in industrial environments. This effect can be reduced if the ANN network is trained with artificially decalibrated spectral data. We are working now with real multi-element scrap samples to check the classification performance.

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