SmartTech-IC 2022

Automatic Selection of Reference Lines for Spectrometer Calibration with Recurrent Neural Networks

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Outline

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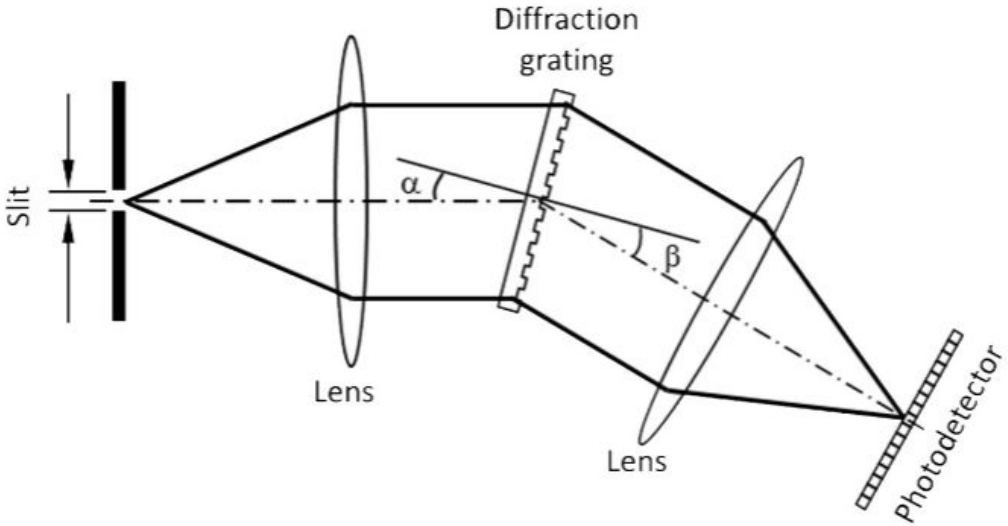
- Problem
- Methodology
- Results
- DEMO
- Conclusions
- Q&A

Basic spectrometer principle

A spectrometer is a scientific instrument used to analyze the light properties of a luminous object, reflected or transmitted light.



Problem

Low-cost spectrometers (~30 USD) < commercial spectrometers (~3000 USD).

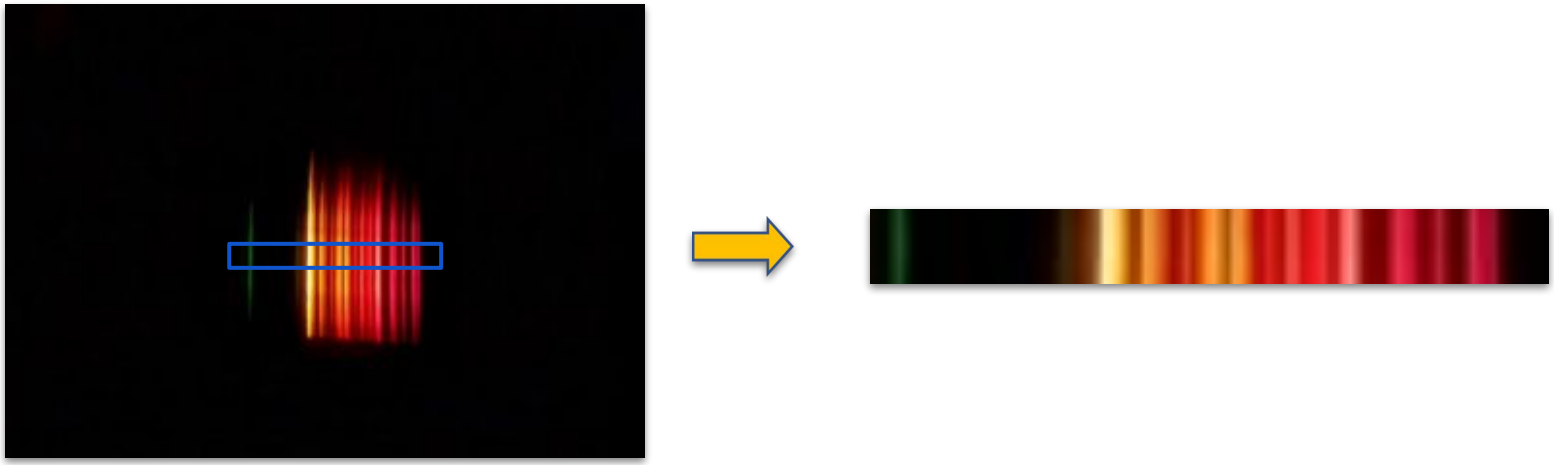
Disadvantages:

- ❑ Selection of reference lines is done manually.
- ❑ Requires to be re-calibrated.

3D-printed low-cost spectrometer

Manual calibration process

1. Select area of interest

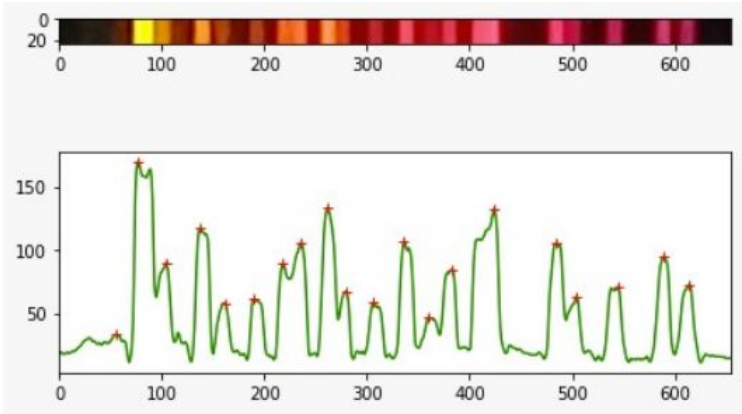


Manual calibration process

2. Get the intensity of each pixel by pre-processing spectra image:

[RGB] => **[Y'UV]** where **Y'=** (0.257×R) + (0.504×G) + (0.098×B) + 16

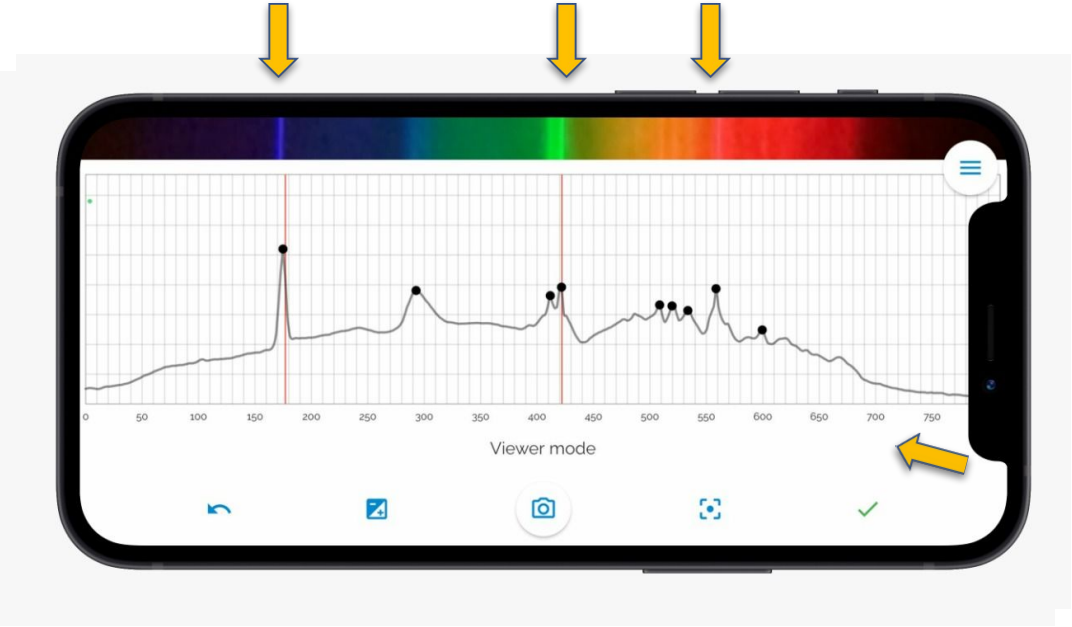
$$intensity_j = \sum_{i=1}^{n} Y'_{i,j}$$



3. Peaks detection

Manual calibration process

4. Selection of reference lines

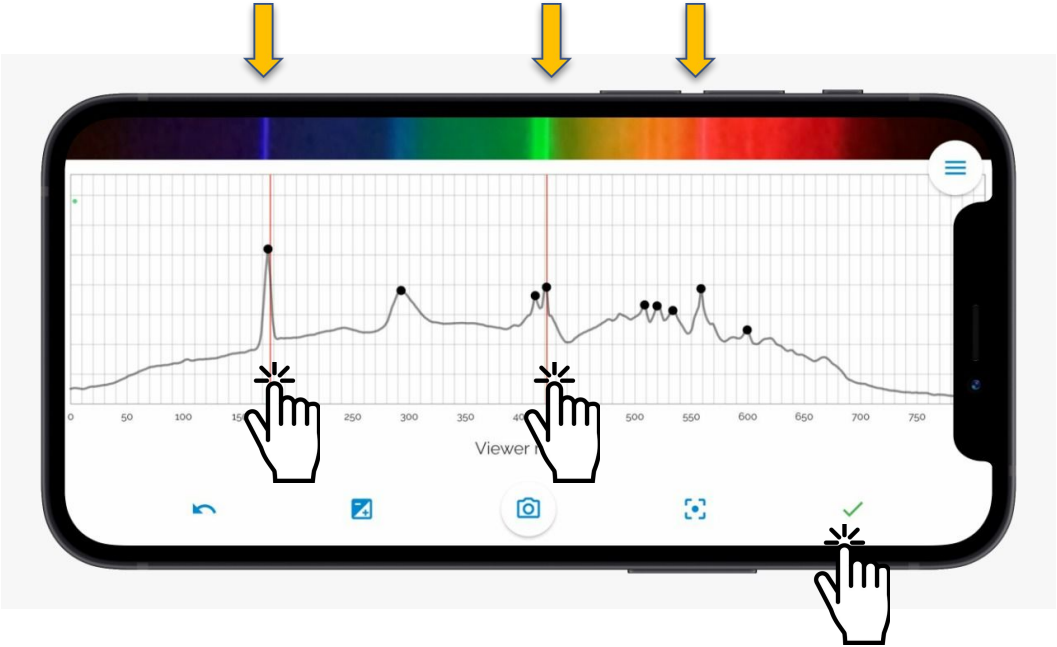


Reference lines - mercury:

# of pixels

Manual calibration process

4. Selection of reference lines



Reference lines - mercury:

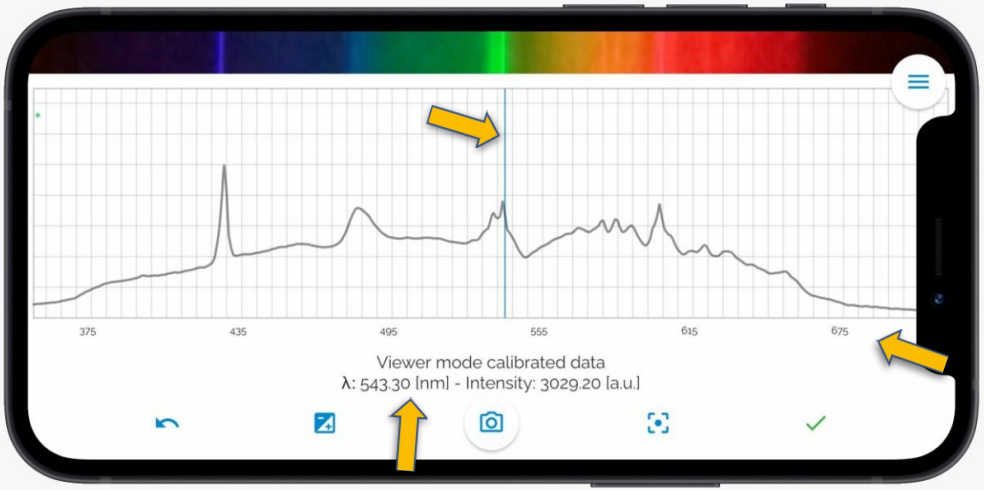
- 435.83 nm
- 546.07 nm

Calibration

Manual calibration process

5. Calibration by fitting a first-order polynomial

$$y = y_1 + (y_2 - y_1) \times \frac{x - x_1}{x_2 - x_1}$$

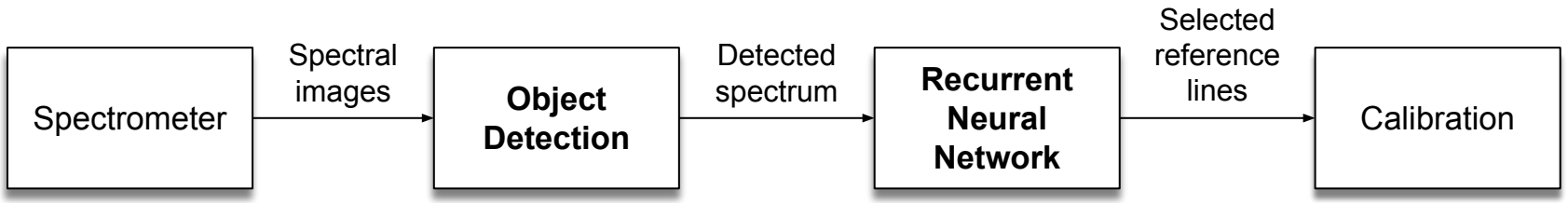


Reference lines - mercury:

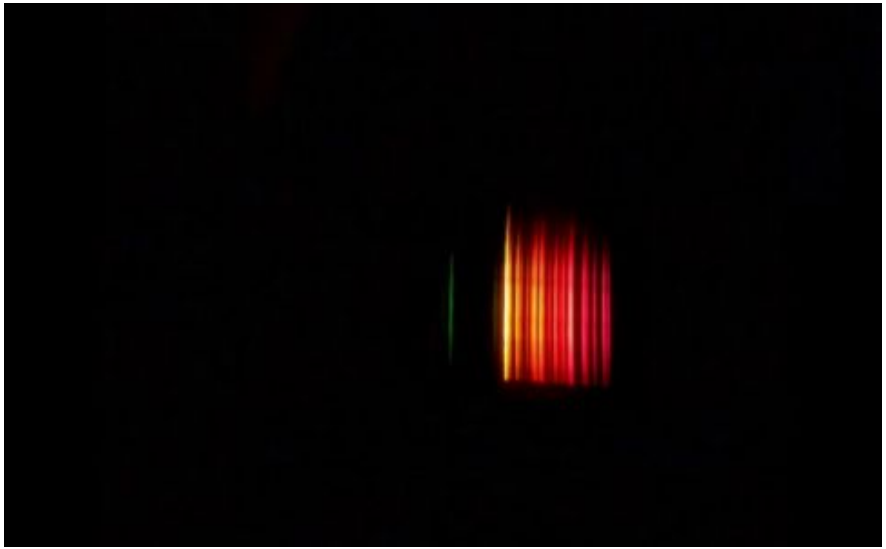
- 435.83 nm
- 546.07 nm

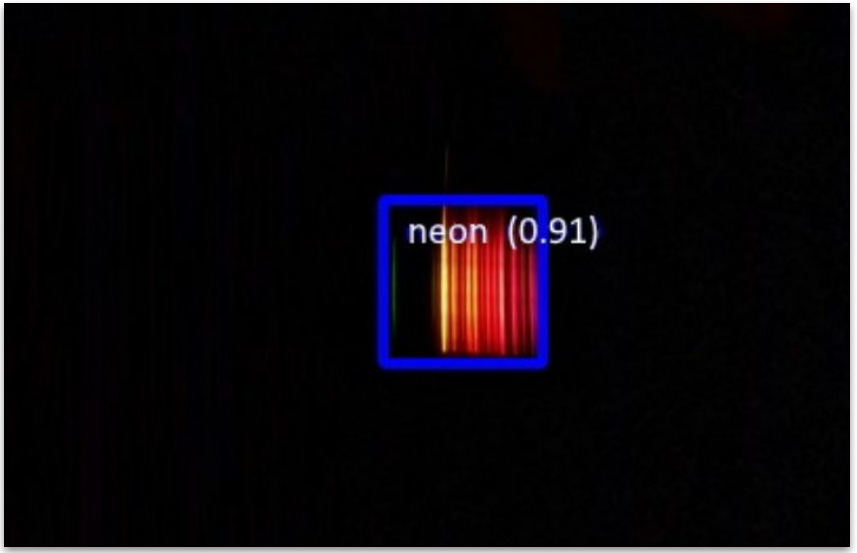
Wavelength [nm]

Methodology

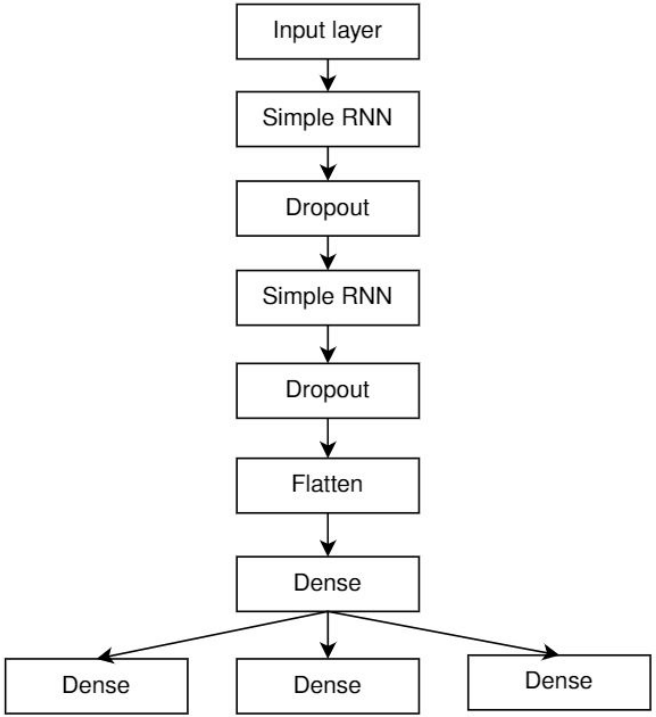


Object Detection





Recurrent Neural Network

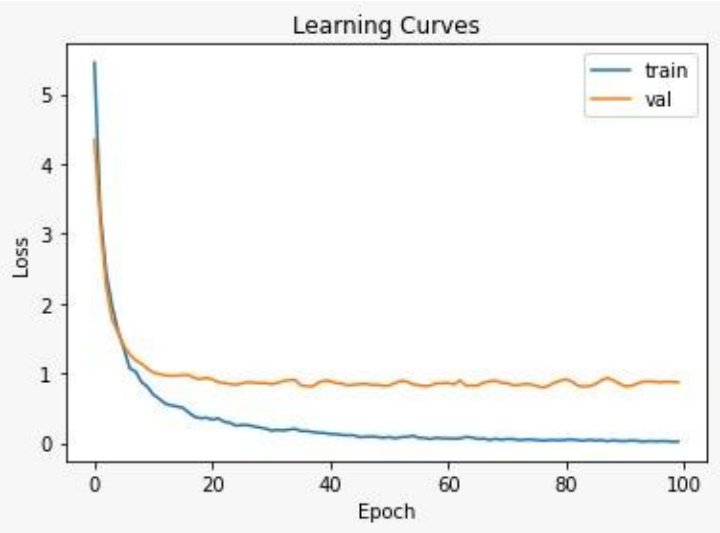


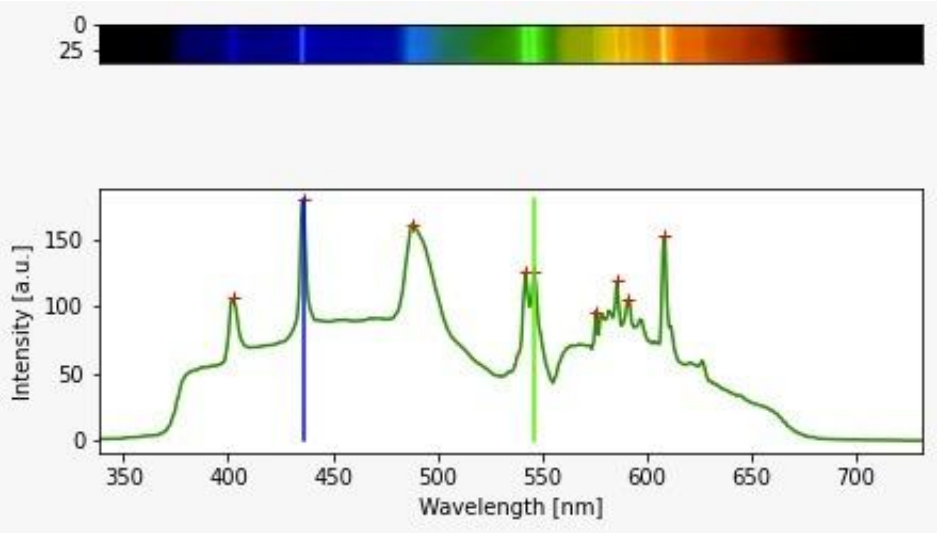
- **Dataset:** 170 neon and mercury spectral images.
- **Labels:** are encoded as the peak index between 1 and 30.

$$L(y_i, \hat{y}_i) = -\sum_{i=1}^{30} y_i * log(\hat{y}_i)$$

Results

Our approach achieves accuracy of **96.97% for the first reference line and 87.88% for the second line.**





Results

Hyperparameter	**Value**
Activation function	*tanh*
Recurrent layers units	20
Dense layer units	192
Learning Rate	0,001
Dropout probability	0,2

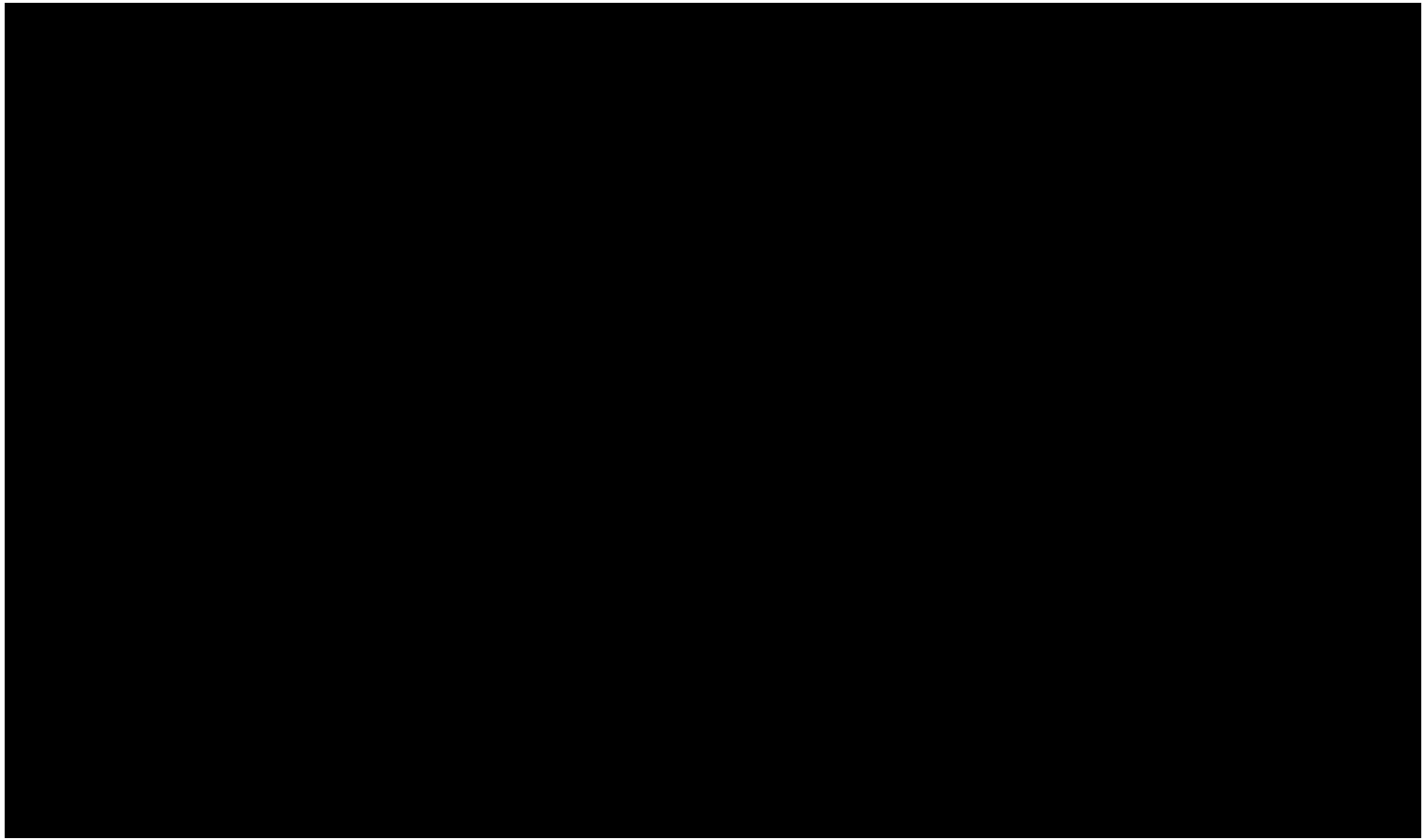
Best hyperparameters found for the calibration RNN model.

Results

We tested our technique and compared the obtained results with NIST Atomic Spectra Database.

Element	Root mean squared error (RMSE)	Mean absolute error (MAE)	Mean absolute percentage error (MAPE)
Neon	0.3919	0.3010	0.048%
Mercury	0.1869	0.1442	0.029%

On average, our measurements have an error of about **0.3 nm for neon and 0.14 nm for mercury.**



Conclusions

- Automate the selection of reference lines for calibrating a spectrometer using recurrent neural networks accurately detect reference lines.
- Allows users to reduce errors and save time by performing automatic calibration using different light sources (e.g., neon and mercury).
- This method suits scenarios that demand remote control such as remote laboratories or applications in which calibration is done frequently.

THANK YOU
Q&A