

LIBSsa: an open source software for analyzing LIBS spectra

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Summary

Laser-Induced Breakdown Spectroscopy (LIBS) is a technique that uses a high-energy pulsed laser to detect and analyze elements present in a sample. The laser beam is directed through an optical system (commonly mirrors, lenses, prisms, or optical fibers) and focused onto the sample's surface. When the laser interacts with the sample, a part is ablated, vaporized, and generates a high-temperature plasma. The species in the plasma emit electromagnetic radiation characteristics of each element in the sample. This radiation is collected by lenses and conveyed through an optical fiber to a spectrometer, where diffraction occurs. The diffracted light is detected using a CCD (charge-coupled device) or ICCD (intensified charge-coupled device). Finally, a spectrum ([Figure 1](#)) is generated ([Miziolek et al., 2006](#)).

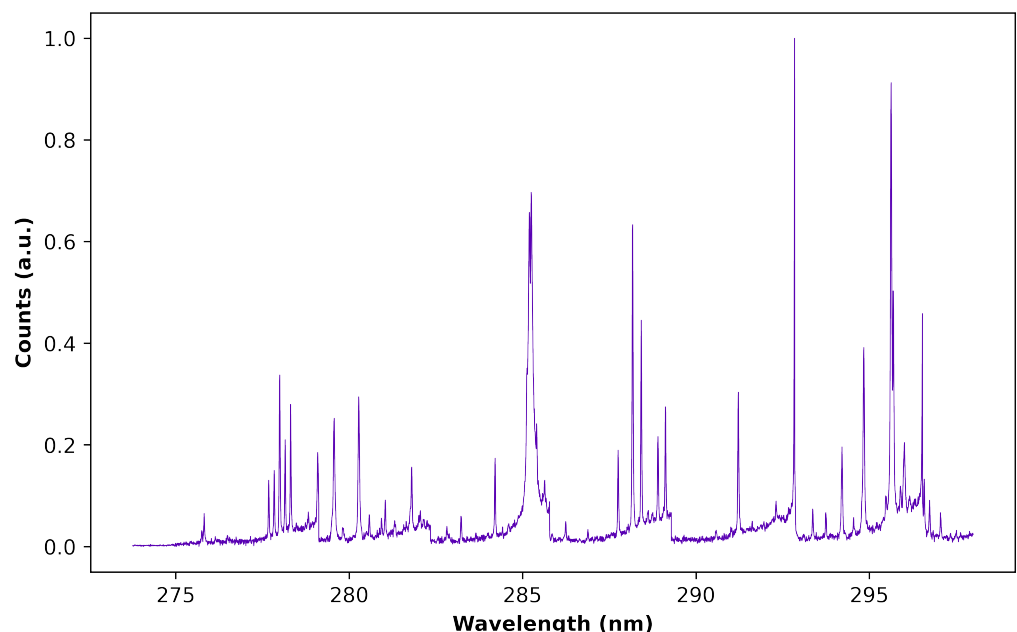


Figure 1: Characteristic LIBS spectrum. Source: self-authored.

Due to its advantages, the LIBS technique has been widely used for elemental characterization in several types of samples, including soils ([Ferreira et al., 2011](#); [Nicolodelli et al., 2014](#); [Stenio, Xavier, et al., 2022](#); [Villas-Boas et al., 2016](#)), leaves ([Ranulfi et al., 2018](#); [Stenio, Costa, et al., 2022](#)), fertilizers ([Marangoni et al., 2016](#)), river sediments ([de Moraes et al., 2021](#)), food ([Vinicius Câmara Costa et al., 2018](#)), metallic alloys ([Noll et al., 2018](#)) and electronic waste

([Vinícius Câmara Costa et al., 2018](#)), to name a few.

The Laser-Induced Breakdown Spectroscopy spectra analyzer (**LIBSsa**) is open-source software written in Python focused on analyzing LIBS spectra. It combines multiple tools used in LIBS analysis into one application, such as outliers removal, isolation of spectral lines, curve fitting, linear models (calibration curves), principal components analysis (PCA), and plasma temperature and electron density calculation.



Figure 2: Logo of LIBSsa. Source: [LIBSsa repository](#).

Statement of need

LIBS measurement is much simpler than other standard elementary characterization techniques, such as Flame Absorption Atomic Spectrometry (FAAS) or Inductively Coupled Plasma Optical Emission Spectroscopy (ICP OES), since it does not require acid digestion for sample preparation. Furthermore, the user can obtain a sample spectrum in seconds. Nonetheless, the analysis of the resulting signal may be highly complex.

Much of the complexity in analyzing LIBS spectra arises mainly due to matrix effects, which hinder the ability to obtain calibration blanks and generate universal calibration curves. As a result, analysts need to adopt various calibration and signal-processing strategies to achieve quantitative measurements.

In general, those working with LIBS commonly develop tools to process the measured signal and extract satisfactory results. However, this practice has the effect of generating highly specialized users of the technique, not only in terms of using instrumentation but also in scientific data analysis tools, such as [R](#), [MATLAB](#), [OriginLab](#), [Weka](#), among others. Although these platforms provide powerful tools for signal analysis, they are not dedicated tools for LIBS spectra analysis.

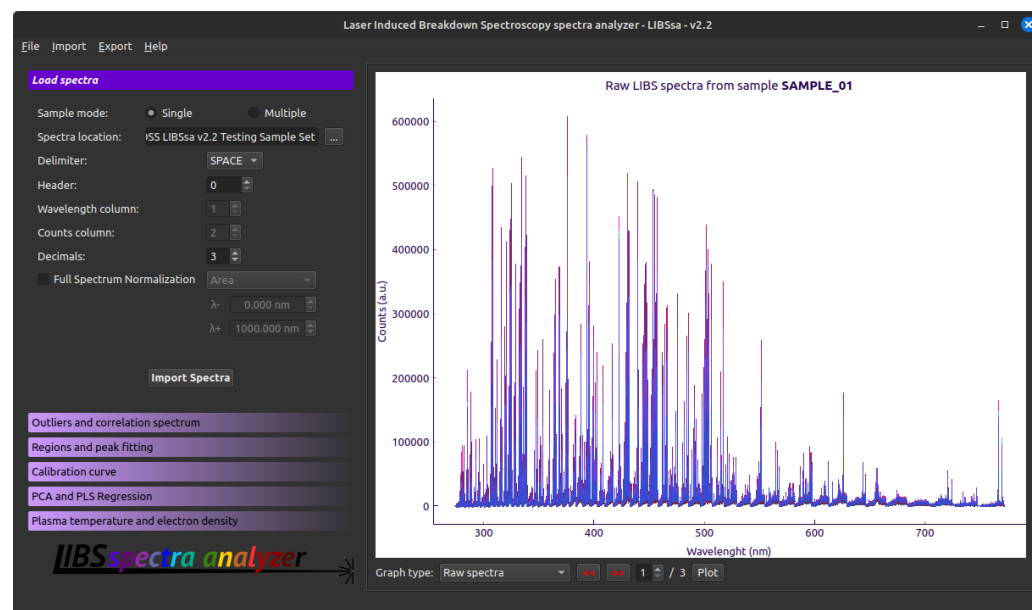


Figure 3: LIBSsa home screen tab with spectra loaded. Source: self-authored.

Knowing about these challenges and aiming to make the LIBS technique more widely used, the authors (Stenio, 2023) proposed a software creation that would automate the LIBS analysis, incorporating strategies used in several works in the literature (Castro & Pereira-Filho, 2016; de Moraes et al., 2021; Marangoni et al., 2016; Nicolodelli et al., 2014; Stenio, Xavier, et al., 2022; Stenio, Costa, et al., 2022). In this way, the LIBSsa software was conceived (Figure 3).

The main purpose of LIBSsa is to help scientists in the LIBS/spectroscopy field gain speed and practicality when analyzing LIBS spectra, allowing fast assessment of which is the best calibration strategy for the sample set.

Brief software description

LIBSsa is straightforward: the user selects the input source (where LIBS spectra are located), loads them into the program, and performs a wide range of analyses, including: removal of outliers using SAM (Keshava, 2004) or MAD (Leys et al., 2013) algorithms, full spectrum normalization (FSN), correlation spectrum, peak isolation, peak fitting (Gaussian, Lorentzian, and Voigt), univariate linear models, multivariate partial least squares regression (PLSR), principal components analysis (PCA), and plasma temperature and electron density calculation using the Saha-Boltzmann equation (Stenio, 2023). Figure 4 shows some of the graphics generated by LIBSsa.

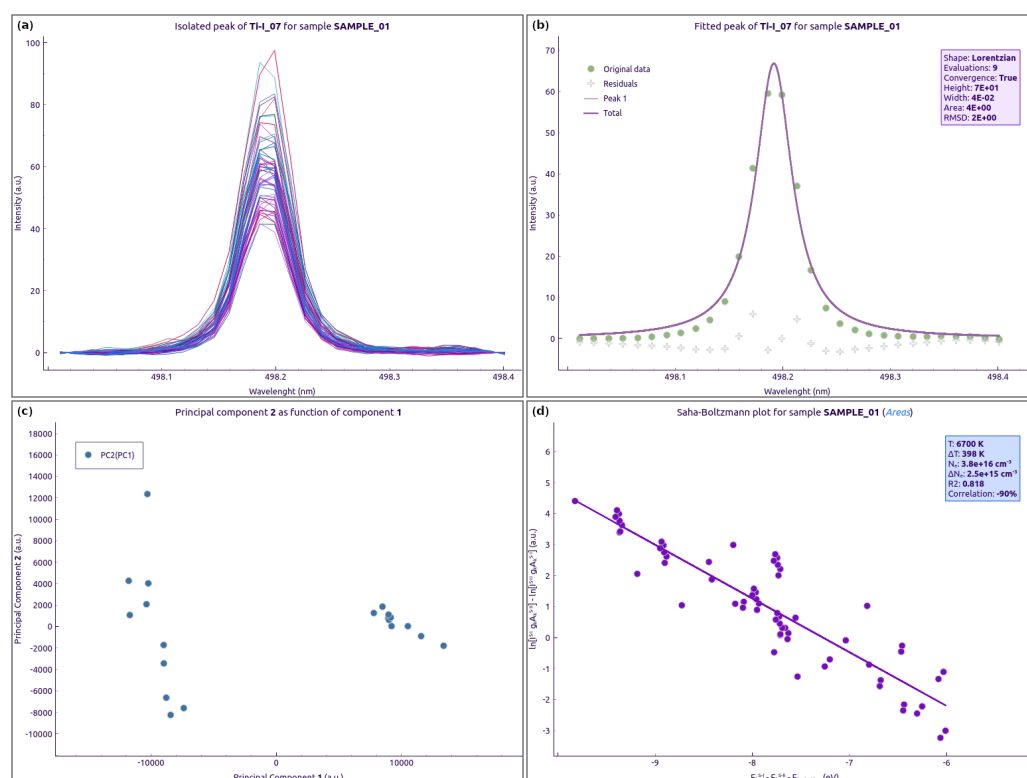


Figure 4: Some analyses available in LIBSsa: peak isolation (a), peak fitting (b), PCA (c), and Saha-Boltzmann plot (d). Source: self-authored.

In each step of the analysis, it is possible to save/export data into multiple file formats (txt, csv, and xlsx). Figure 5 shows a typical LIBSsa analysis workflow.

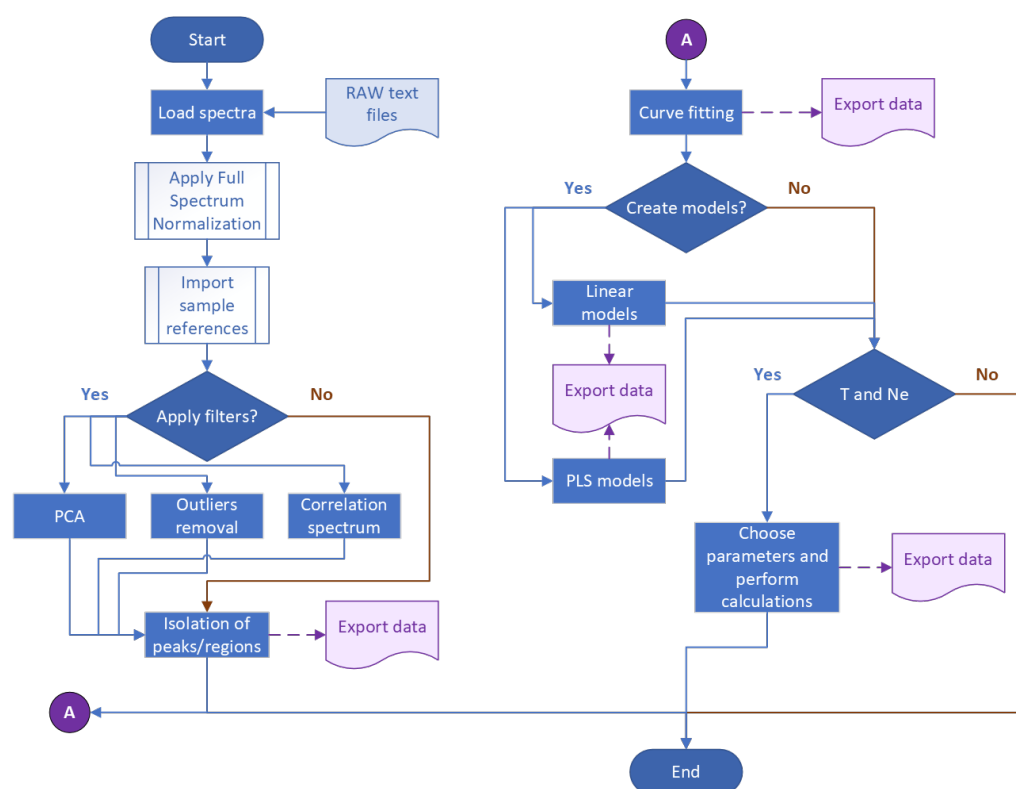


Figure 5: LIBSsa working flowchart. Source: self-authored.

In order to properly operate, the program uses the libraries **NumPy** (Harris et al., 2020) and **SciPy** (Virtanen et al., 2020) for most calculations, **pandas** (McKinney & others, 2010) and **openpyxl** (Team of developers of Openpyxl, 2023) to export spreadsheets, **scikit-learn** (Pedregosa et al., 2011) to fit linear, PLS and PCA models, **pyqtgraph** (Team of developers of PyQtGraph, 2023) to show in program graphics, and finally **PySide6** (The Qt Company, 2020) as the graphical user interface (GUI) framework.

Author contributions

Conceptualization: K. S., D. M. B. P. M.; data curation: K. S.; formal analysis: K. S.; funding acquisition: D. M. B. P. M.; investigation: K. S.; methodology: K. S.; project administration: K. S.; resources: D. M. B. P. M.; software: K. S.; supervision: D. M. B. P. M.; validation: K. S., D. M. B. P. M.; visualization: K. S.; writing – original draft: K. S.; writing – review & editing: K. S., D. M. B. P. M.

Conflicts of interest

There are no conflicts to declare.

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