P5

Fitting LIBS plasma using gradient descent

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The calibration-free LIBS (CF-LIBS) method enables the determination of quantitative plasma parameters without the need for calibration data. This can be especially useful in contexts where there is no - or not enough – matrix-matched data, such as in in-situ rover missions. Besides the indirect CFLIBS methods where plasma parameters are inferred from the spectrum directly [1], there is also the direct method where an experimentally obtained LIBS spectrum is compared to a synthetic spectrum produced by the simulation of a feasible plasma model [2].

In this work we have implemented a plasma model that is differentiable via autodifferentiation with respect to all of its parameters (e.g. temperature, elemental concentrations). We present a fitting scheme that utilizes gradient descent to find the optimal plasma parameters. Using gradients enables a speed up with respect to the "black-box" Monte-Carlo method presented in [3].
At the same time our method does not require previous expert knowledge of the target, such as selecting suitable transitions, and is able to optimize all plasma parameters simultaneously instead of iteratively [4].
In the specific case of our model, a homogeneous one-dimensional plasma at local thermal equilibrium, we demonstrate that the gradient descent approach is able to find the optimal solution fast and consistently. We show that this approach is generic and can be extended to more complex plasma models.

Keywords: Gradient Descent; Calibration-Free LIBS; Optimization;

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