A Bayesian Approach to Estimating Fire Emissions from FTIR Time Series

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Introduction

* An accessible Python framework for measuring common and trace gas emissions from an **FTIR time series** is presented here.
* The model produces **concentration estimates**, alongside the **uncertainties** implicit in emission estimation.
* It can also be used to understand the **correlation** between the concentrations of different chemical species emitted, which could be useful when comparing the burns of different materials, e.g. peat and straw.
* The model improves on other algorithms by encoding the assumption that the concentration of a given chemical species doesn't change drastically between adjacent time steps.
* We can implement this assumption into a **Bayesian regularisation term**, which considers the concentration estimates of the chemical species at the proceeding two time steps.
* The model has the potential to measure the emissions of >60 chemical species simultaneously.
* Better quantification of trace gas emissions could be useful in understanding different different burn regimes. Formaldehyde, NO_x, and SO_2 are particularly important, for example, when considering peat burns.

Methodology

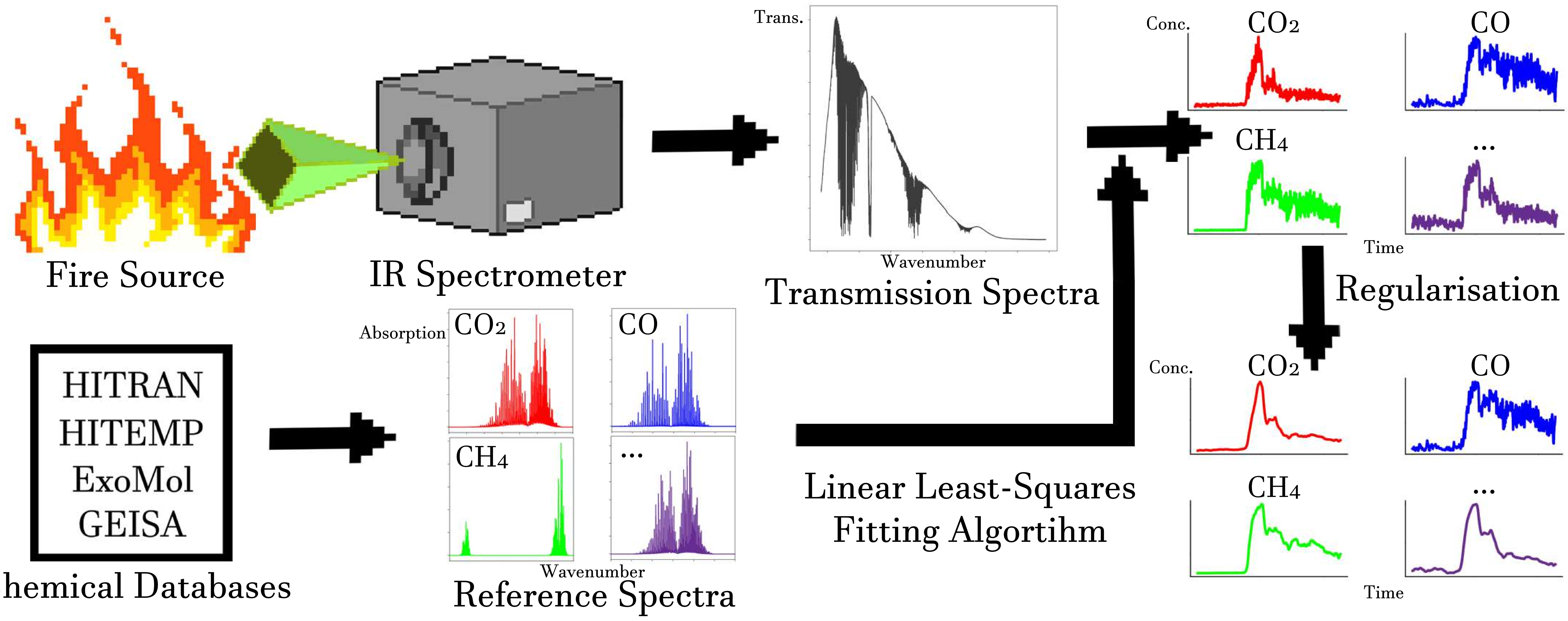
* The transmission spectra from a fire are measured by an IRcube FTIR Analyser.
* From this, the **absorption spectrum** of each individual time step can be derived.
* Reference absorption spectra for individual chemicals are pulled from the HITRAN, HITEMP, ExoMol, and GEISA databases and are broadened to user-inputted temperature and pressure measurements.
* A matrix of reference absorption profiles for each chemical is then fit to the absorption spectrum at each time step using a **linear least-squares fitting algorithm**.

$$\underbrace{\text{Absorption Spectrum}}_{A} = \sum_{j=1}^{N_s} \underbrace{\text{Weight}}_{\nu_j} \cdot \underbrace{\text{Reference Spectrum}}_{\beta_j}$$

* Where N_s is the total number of species and ν represents the concentration of each chemical - which we solve for.
* We can apply a **Bayesian regularisation term** our results. From this we can refine our estimation of the concentration for each species over time.

$$\underbrace{\nu(t_{\text{step}}) - 2\nu(t_{\text{step}}+1) + \nu(t_{\text{step}}+2) \sim 0}_{\text{Condition for Bayesian regularisation}}$$

* We assume the concentration at a specific time step is approximately equivalent to that at the proceeding two time steps.



Future Development

* The model will be implemented on two series of burns, one on Canadian peat samples and the other on straw.
* Using these burns, model outputs will be **validated** on the outputs of the proprietary software, OPUS GA.
* A full study of how different chemical species correlate with each other through the burns will be conducted.
* We will investigate the potential for understanding how trace gases correlate with other trace gas species during combustion.
* The range of chemicals used in the model will be expanded.
* However, adding more chemicals could pose issues for the uncertainty in the estimates and add significantly to the time needed to produce emissions estimates.
* Iteration on the how significant the Bayesian regularisation term should be for accurate results will be tested.
* We intend to publish this model, with its code accessible in a public repository, for wider use “soon”...

References

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