Real-time parameter inference in reduced-order flame models with heteroscedastic Bayesian neural network ensembles

Background

- Estimating unknown model parameters with uncertainties from observed data can be an expensive inverse problem.
- Neural network-based amortized inference techniques learn surrogate of the approximate posterior $p(\theta | \mathbf{z})$, can be rapidly evaluated.

The G-equation model

Positive feedback in interactions between flames and acoustic waves can result in devastating thermoacoustic instabilities in jet or rockets engines.



The G-equation is a kinematic reduced-order model that describes flame response to acoustics. It models the flame as an infinitely-thin front propagating into unburnt gases at a fixed speed s_L . The flame front is defined as the G = 0 contour of the two-dimensional time-varying G-field G(x, y, t).

$$\frac{\partial G}{\partial t} + \mathbf{v} \cdot \nabla G = s_L |\nabla G|$$

Any flame dynamics that can be generated by the G-equation may be uniquely specified by a set of 6 parameters θ which we need to infer from experimental observations: K, ϵ_a , M_k , v_a , St and β .

Ensemble Kalman filter suggested in the literature [Yu et al.] takes O(hours) and needs a long sequence of observations to converge to a parameter estimate; can converge to bad local optima.

Conclusions

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Tool: heteroscedastic Bayesian Neural Networks

We assume that the posterior over parameters θ given observations \mathbf{z} , $p(\boldsymbol{\theta}|\mathbf{z})$ can be modelled as a Bayesian neural network $\boldsymbol{\mu}(\mathbf{z};\mathbf{w})$ with heteroscedastic Gaussian aleatoric uncertainty $\sigma(z; w)$. The epistemic uncertainty of the Bayesian surrogate detects flame observations that are either not within the parameter range of the training dataset or cannot be modelled by the G-equation.



The size of the dataset calls for scalable approximate inference techniques for training the neural network. Here we use approximately Bayesian ensembling using randomized maximum a posteriori (MAP) sampling [Pearce et al.].

Data: experiments

Our apparatus has a premixed laminar Bunsen flame inside an enclosure, with an optical access window for a high-speed camera. A loudspeaker is mounted upstream of the flame for acoustic forcing.



Experiments were performed at different fuel compositions (methane: ethene ratios), flow rates, excitation frequencies (250 - 450 Hz) and excitation amplitudes.

Thresholding is applied to detect the flame front. We divide the domain vertically into 90 horizontal strips and compute the flame area corresponding to the flame segment it contains. Each frame is thus converted into a 90-dimensional vector of flame areas. 10 successive frames from a video recording are stacked to form an observation \mathbf{z}_i .

Heteroscedastic Bayesian neural network ensemble used to calibrate parameters of the G-equation, a reduced-order model for predicting the acoustic response of premixed flames. Trained and tested on millions of simulated flame videos, G-equation parameters can be accurately recovered with uncertainties for simulation data. Applied to experimental high-speed video footage of acoustically excited flames to recover parameters accurately, in real-time, from very short sequences of flame observations.

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Data: simulations

For the simulation dataset, we sample from the prior $P(\theta)$, assumed uniform within the hyper-rectangle defined by bounds $0 \le K \le 2.5, 0 \le \epsilon_a \le 1.0$, $0.02 \le M_k \le 0.08, 0.0 \le v_a \le 1.0, 0.5 \le St \le 125.0, 2.0 \le \beta \le 10.0$ and $0.08 \le f_s \le 0.20$. For each sample, the G-equation is solved using LSGEN2D and the solution is time marched until a limit cycle is reached. Simulated flames then undergo the same data pre-processing steps as the experimental flames to create a dataset with 2.4 million simulated flame observations.

Results

Results on the test set of simulated observations (Figure 3) indicate that accurate estimates of G equation parameters are recovered by the neural network. The correlation coefficient ρ between true and predicted parameter values are 0.982, 0.994, 0.971, 0.993, 0.976 and 0.990 for K, ϵ_a , M_k , v_a , St and β , respectively. Estimates of parameter uncertainty are also well-calibrated.



We use the trained network to predict parameter values for 10 experimental flame videos and re-simulate the flames using predicted parameter estimates. The re-simulated flames match the dynamics of the real flames closely.



