Non-uniform combustion temperature estimation using laser absorption spectroscopy and Multi Output Gaussian Process Regression

Saumya Vilas Roy, saumyaroy@tutanota.com

Guided by

Rajesh Sadanandan
Associate Professor (Aerospace Department)

Deepak Mishra
Professor (Avionics Department)

Satheesh K.
Associate Professor (Aerospace Department)

Indian Institute of Space Science and Technology (IIST)

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Introduction

- ML transforms industries by enabling computers to learn from data and make predictions autonomously.
- GPR, a versatile and potent ML technique, models intricate data relationships effectively.
- Being a Bayesian non-parametric method, GPR captures uncertainties and offers detailed probabilistic results.
- Suitable for regression, classification, and optimization, GPR finds applications across diverse fields.
- Applying GPR's capabilities, the research estimates the non-uniform temperature profile in a simulated combustion system.

Applications of Gaussian Process Regression (GPR)

- It enables precise prediction of continuous values with uncertainty estimates.
- It effectively captures trends and irregularities in time series data.
- It utilizes uncertainties to optimize parameter values efficiently.
- It proficiently detects anomalies by modeling normal behavior.
- It plays a significant role in motion planning and adaptive control in robotics.
- It offers efficient computational cost reduction in simulations and optimization.

Multi-output Gaussian Process Regression (MOGPR) extends Gaussian Process Regression (GPR) to model multiple correlated outputs simultaneously, beneficial for interrelated tasks.

- MOGPR models relationships between multiple outputs.
- Leverages shared information for more accurate predictions.
- Captures underlying structure for compact data representation.
- Enables transfer learning between related tasks.
- Used in neuroscience, environmental modeling, bioinformatics, robotics, etc.

Importance of Combustion Diagnostics

- Diagnosis helps optimize combustion processes for better energy efficiency.
- Identifying combustion issues can lead to lower emissions, benefiting the environment.
- Early detection of combustion problems can prevent equipment damage and prolong its lifespan.
- Ensuring proper combustion reduces the risk of accidents and improves workplace safety.
- Efficient combustion reduces fuel consumption and operational costs.

Importance of Temperature Profiles

- Temperature influences the kinetics of chemical reactions in combustion processes.
- Temperature profiles provide insights into the distribution of heat within a flame.
- Temperature profiles can help predict flame behavior, including ignition, propagation, and extinction.
- Deviations in temperature profiles can indicate anomalies or inefficiencies in combustion processes.
- Temperature profiles serve as valuable data for validating computational models of combustion.

Estimating Non-Uniform Temperature Profile using MOGPR

- We aim to estimate the non-uniform temperature profile of a combustion system by parameterizing it as a Boltzmann distribution.
- Gaussian process regression has emerged as a valuable tool for modeling and predicting flame characteristics with high accuracy and efficiency.
- By leveraging the flexibility and non-parametric nature of Gaussian processes, researchers have been able to extract valuable insights from complex flame data.
- This paper explores the combined application of TDLAS and Gaussian process regression in flame diagnostics, highlighting its potential to revolutionize the analysis and interpretation of flame behavior.

Theory behind GPR

Definition: A Gaussian process is a collection of random variables, any finite number of which have a joint Gaussian distribution.

- A Gaussian process is a generalization of the Gaussian probability distribution.
- It is a distribution over functions rather a distribution over vectors.
- It is a non-parametric method of modeling data (i.e. It doesn’t assume any distribution for the data).
- A Gaussian Process is of infinite dimensions. However, we only work with a finite subset.
- Covariance function defines the properties in the function space.
- Data points ”anchor” the function as specific locations.

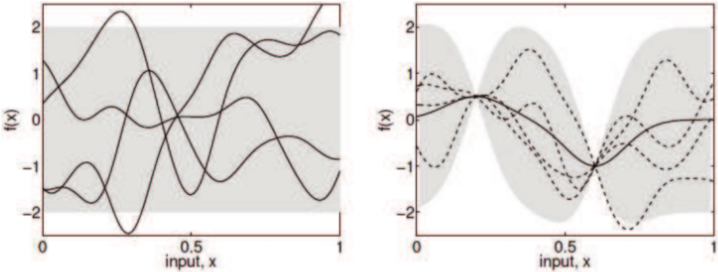


Figure: **Left** Samples drawn from the prior distribution of functions with no observed datapoints. **Right:** Samples drawn from the prior distribution of functions with two observed datapoints. Solid black line shows the mean and shaded region twice the standard deviation.

Introduction to Multi Output Gaussian Process (MOGPR)

The conventional Gaussian Process Regression (GPR) maps only a single distribution but in cases where we need to map two distributions together for example non uniform T and mole fraction of the absorbing species x_i we need to expand it so it can handle multiple outputs.

There are several ways it can be achieved by:

- Parallel single output GPRs
  It is just using multiple single output GPRs in parallel to estimate the each individual point in output distribution (i.e. Assuming all the points in output are independent.)
- MOGPR- Linear Model of Coregionalization (LMC)
- MOGPR - Intrinsic Coregionalization Model (IMC)

MOGPR - Linear Model of Coregionalization (LMC)

It works by allowing several independent samples from GPs with different covariances and talking their weighted sum to model the output distribution.
For an output $f_d(x)$

$$f_d(x) = \sum_{q=1}^{Q} \sum_{i=1}^{R_q} a^i_{d,q} u^i_q(x)$$

Here
$u^i_q(x) \sim \mathcal{GP}^i_q(0, k(x, x^{'}))$
Q number of groups.
R_q is number samples in a group.

MOGPR - Intrinsic Coregionalization Model (ICM)

It works by take a single sample from GP and talking their weighted sum to model the output distribution.
For an output $f_d(x)$

$$f_d(x) = \sum_{i=1}^{R} a_d^i u^i(x)$$

Here
$u(x) \sim \mathcal{GP}(0, k(x, x^{'}))$
Q number of groups.
R_q is number samples in a group.

Basics of Spectroscopy

- Spectroscopy studies matter through its interaction with different frequencies of the electromagnetic spectrum.
- It is a versatile methodology used to extract various information such as energies of electronic states, molecular structure, and dynamic information.
- Spectroscopy observes light's interaction with molecules' degrees of freedom, providing different pictures or spectra based on the light frequency used.

Interaction of light with a medium can influence the sample and/or the light. Method involves: (1) excitation and (2) detection.

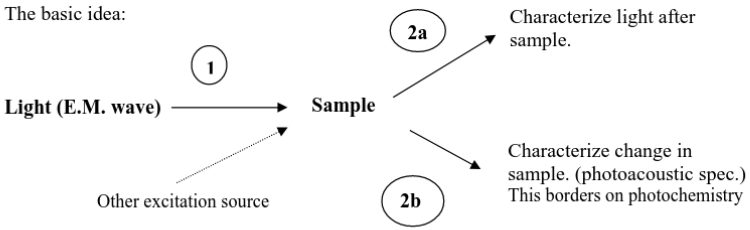


Figure: Block diagram of Spectroscopy.

LASER absorption Spectroscopy

1) Absorption: Change in intensity I_o of incident light as it passes through a medium.
Transmission $\tau_v = I/I_o$

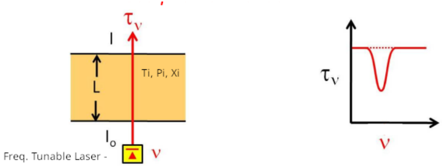


Figure: Absorption of monochromatic light.

- Line-of-sight direct absorption
  - Beer-Lambert relation $\tau_v = \frac{I}{I_0} = exp(-k_v.L)$
  - Spectral absorption coefficient $k_v = S(T).\Phi(T, P, \chi_i).\chi_i.P$
  - Assumes an uniform temperature profile in the medium.

Absorption Spectra

- In figure: absorption spectra of a molecular species of interest to combustion systems.
- Line-strength $s(T)$ depends on Temperature T, Pressure P,Mole fraction X_i and Pathlenght L.

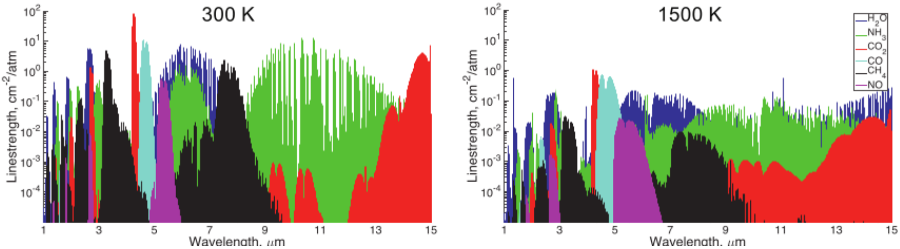


Figure: Linestrengths (i.e., absorption strength) of several molecular species of interest to combustion systems for a fixed X_i at two different temperatures.

- From the above absorption spectrum, for the molecule of interest (in the case water vapor H_2O), the absorption transition which is sensitive to temperature changes is selected for the laser diagnostics experiments using DAS.
- Experiments are performed to capture the molecular absorption spectrum through the medium of interest (Fig. 2.2, right).
- After selecting the absorption line. The objective is to find the non-uniform temperature profile inside the region of interest using the line absorbance information.
- The Beer-Lambert law above assumes a uniform temperature profile. However in real combustion systems profiles could be like as follows but they can take any shape or form (Non-uniform temperature profile inside the medium).

Temperature profile inside a combustion system

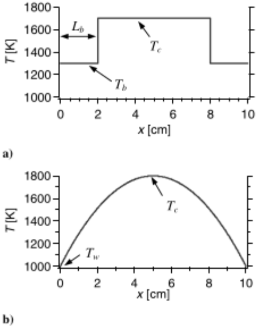


Figure: Postulated non-uniform temperature distribution profiles for confined combustion gases with cold walls.

In addtion the mole fraction of the absorbing species xi can also have a non-uniform distribution though the medium. In the present study the goal is to estimate their non- uniform temperature profile from the measured molecular absorption spectrum using DAS assuming a constant xi through the medium.

Methods to estimate temperature profile

- Fixed wavelength: Laser operates at a constant wavelength resonant with a molecule's absorption transition (Direct absorption) or modulated around a fixed wavelength (Wavelength-modulation spectroscopy).
- Scanned wavelength: Laser wavelength scans across a portion of the molecule's absorption transition, accompanied by simultaneous high-frequency sinusoidal modulation in Wavelength-modulation spectroscopy (WMS).

One possibility to estimate the temperature profile from the DAS measurement data is using Radon transform.

- Radon transform:

  It is the integral transform which takes a function f defined on the plane to a function Rf defined on the (two-dimensional) space of lines in the plane, whose value at a particular line is equal to the line integral of the function over that line.

  Drawbacks:

  It required a lot of lines or data points to estimate the shape or the curve of underling profile.

Experimental Setup

The experimental setup is designed as such to get a non uniform temperature field while maintaining an uniform mole fraction (Xi) throughout the laser path.

- For this a stainless steel tube with a 1cm hole for passing the laser through was kept in a heated three zone furnace.
- Three K type thermocouples are used to monitor the temperature in the middle portion of the cell. at a pre-set value.
- The temperature then gradually goes down to room temperature as it comes to the exit of the cell.
- A DFB laser centered at the molecular absorption transmission of H2 O molecule at 1343.3 nm is used in the experiment to generate the absorption spectrum.

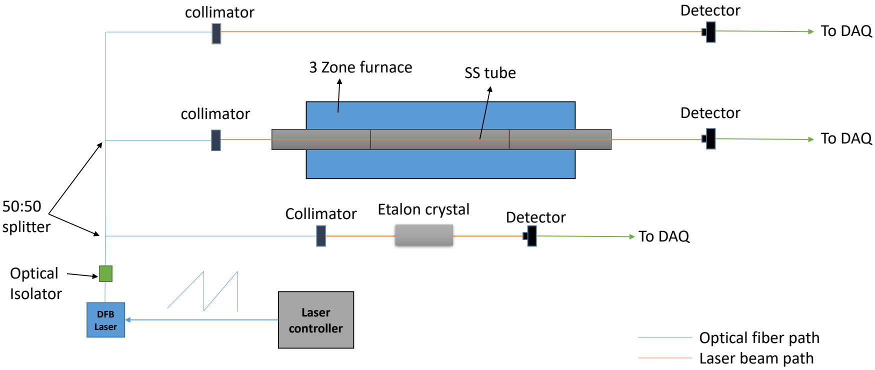


Figure: Schematic of tube in the furnace.

- To capture the full line profile of the absorbing line; The laser current is modulated using a laser current controller at a frequency of 1Khz.
- The laser beam path is split into three. One path for wavelength calibration of the laser using an etalon crystal.
- One for getting a reference spectrum at ambient conditions and the third path passes through the heated cell.
- The resulting laser beam intensity after absorption by the H_2O molecule in the heated cell is collimated using a doublet and detected using a photodetector.
- The detector signal is post processed and absorption spectrum is obtained.

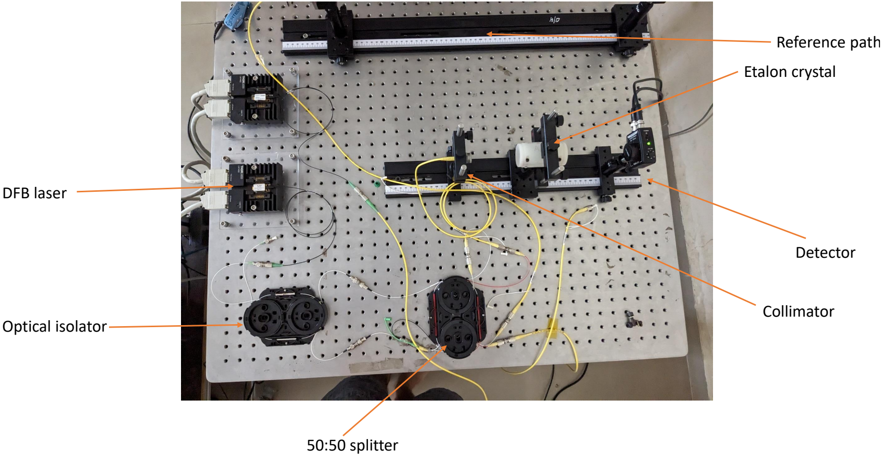


Figure: DFB laser setup.

Process flow chart

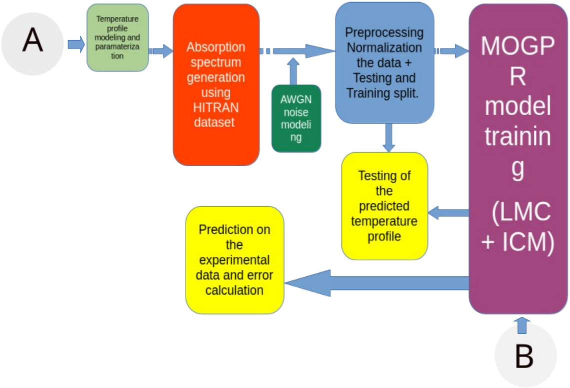


Figure: Flow chart of MOGPR model.

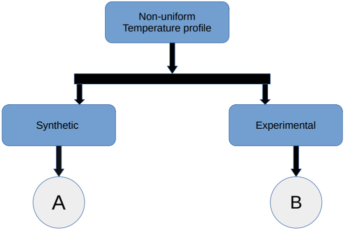


Figure: Data modeling.

- Temperature profile modeling and parameterization.
- Absorption spectrum generation using HITRAN dataset.
- AWGN noise modeling for simulating real-world noise.
- Preprocessing: Data normalization and testing/training split.
- MOGPR model training (LMC + ICM) for regression.
- Testing predicted temperature profiles for accuracy.

Dataset modeling

- Spectral dataset sourced from HITRAN database for H_2O molecule.
- Water Vapor (H2O) selected as the species of interest for absorption study.
- Absorption observed in the wavelength range 7443.9 to 7445.1 cm^{-1}.
- Training data generated using simulated Boltzmann temperature profile with 3 variables.
- Features generated using HITRAN database for absorption spectrum.
- Mole fraction of the species assumed constant at 0.026.
- Pressure: 1 bar, Ambient temperature: 303 K, Path length: 110 cm.
- Total dataset samples generated: 7000.

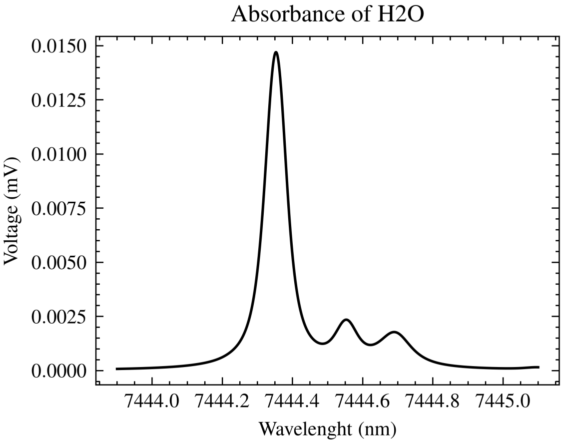


Figure: The absorbance of H2O in the given wavelength limits.

Noise modeling

- Simulated noise added to the absorbance to mimic real-world conditions.
- Signal to Noise Ratio (SNR) calculated for a test experimental signal.
- Additive White Gaussian Noise (AWGN) added to the absorbance signal based on the SNR.
- Value of SNR: 33.5505.

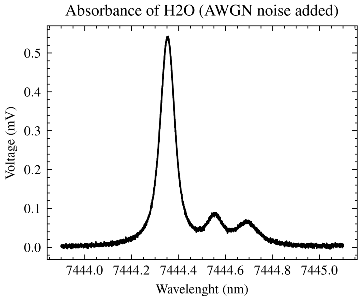


Figure: The absorbance of H2O in the given wavelength limits (With AWGN noise added).

Modeling Non-Uniform Temperature Profile

The non-uniform temperature profile in a high-temperature system was modeled using a Boltzmann fitting profile to reduce prediction overhead and parameterize the temperature profile effectively.

$$y = A_2 + \frac{A_1 - A_2}{1 + e^{(x - x_0)/A_3}}$$

Where:

- y: Flame temperature
- A_1: Central uniform temperature
- A_2: Ambient temperature (Room temperature)
- A_3: Describes the level of transition gradient
- x_0: Radial position where flame temperature is $(A_1 - A_2)/2$

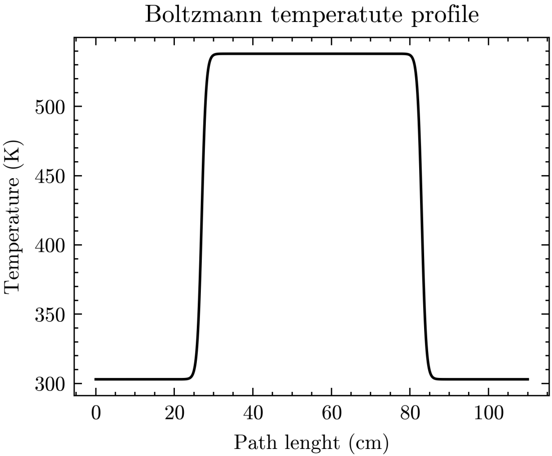


Figure: The modeled Boltzmann temperature profile.

Multiple profiles can be generated by changing values of parameters in equation above
A_1 is varied from 303 K to 773 K.
$A_2 = 303$ K as the ambient temperature.
A_3 is varied from 1 to 10.
x_0 is varied from 0 to 55 (simulating half of the pathlenght of the burner).
These three variables $A_1, A_3 \& x_0$ are varied to generate multiple test and training temperature profiles.

MOGPR Modeling

- **Utilization of GPy**: GPy, a Python library by SheffieldML, addresses challenges in MOGPR modeling with Gaussian processes.
- **Data Normalization**: StandardScaler from SciPy normalized the data for standardized feature scaling.
- **LMC and ICM Techniques**: LMC and ICM enable modeling correlations between multiple parameters and features.
- **Model Saving and Reloading**: Pickle module in Python used for saving and reloading models and variables.
- **Feature and Target Data**: Absorbance spectrum [1x3000] used as a feature for MOGPR models to predict temperature profile parameters [1x3].
- **Choice of Kernel**: Radial Basis Function (RBF) used as the kernel function for capturing complex patterns.
- **Model Convergence**: Training continued until models reached a stable state for optimal performance.

Loss Functions

- **RMSE Maximum (**$RMSE_{max}$**)**: Calculates the maximum RMSE value across all test profiles.
- **RMSE Minimum (**$RMSE_{min}$**)**: Assesses the minimum RMSE value across all test profiles.
- **RMSE Average (**$RMSE_{avg}$**)**: Computes the average RMSE value across all test profiles.

$$RMSE_{max} = MAX_H(\sqrt{\sum_{i=1}^{D}(x_i - y_i)^2})$$

$$RMSE_{min} = MIN_H(\sqrt{\sum_{i=1}^{D}(x_i - y_i)^2})$$

$$RMSE_{avg} = \frac{1}{H}\sum_{i=1}^{H}(\sqrt{\sum_{i=1}^{D}(x_i - y_i)^2})$$

Methodology

Both AWGN modeled noise added and noise free simulated data were used to train MOGPR models.
7000 total data points were generated for each case which was further split **80:20** for training and testing in MOGPR
Total training data samples: **5000**
Total testing data samples: **2000**
Both ICM and LMC MOGPR methods were used and with two noise variations total 4 models were trained as follows.
Table 1 shows the models trained.

Table: MOGPR Model List

Models	Methods	Noise
α MOGPR	LMC	Noise Free
β MOGPR	LMC	AWGN Noise
γ MOGPR	ICM	Noise Free
θ MOGPR	ICM	AWGN Noise

Results

Table 2 shows the models tested on the generated dataset.

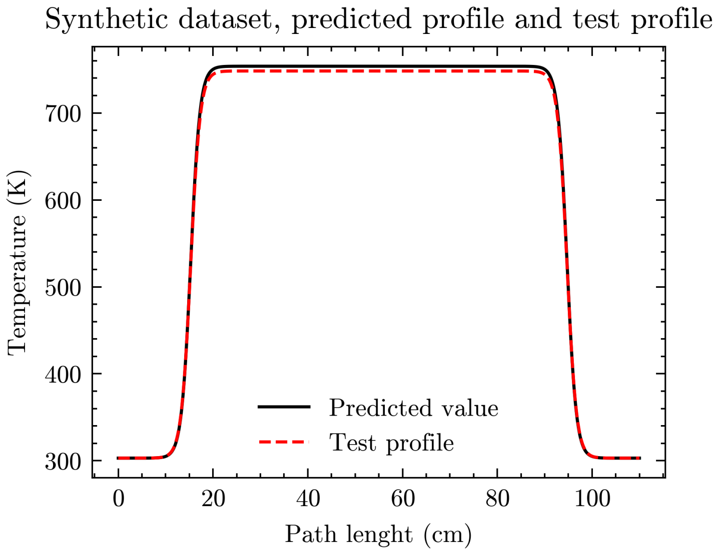
Table: MOGPR Model Testing Error

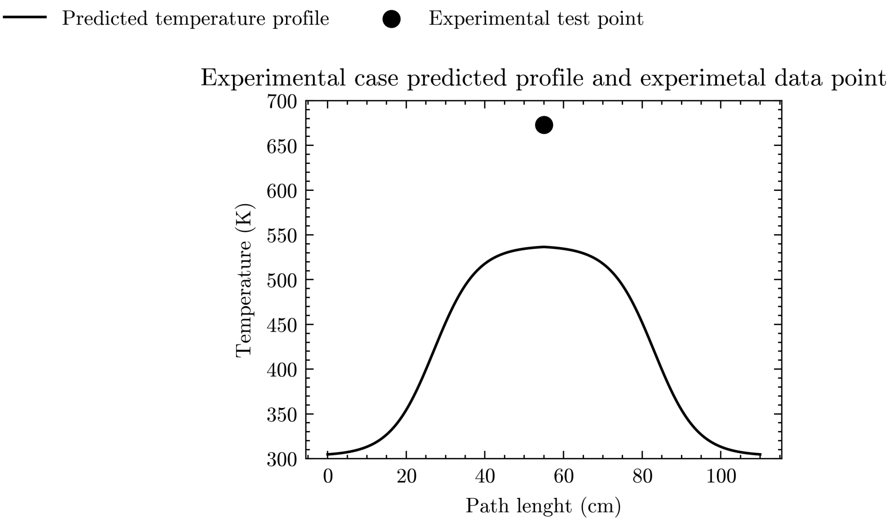
Models	$RMSE_{max}$	$RMSE_{min}$	$RMSE_{avg}$
α MOGPR	458.5093	0.1938	22.3659
β MOGPR	87.7101	4.4214e-04	19.9165
γ MOGPR	410.5743	0.0965	27.7380
θ MOGPR	82.8912	7.923e-05	20.2450

Table 3 shows the models tested on the experimental data point. As measurement of the entire temperature profile inside the heated cell was not possible, only the peak flame temperature were compared and the percentage difference show in the table below

Table: MOGPR Model Testing Error

Models	**Error (%)**
α MOGPR	20.0594
β MOGPR	20.0593
γ MOGPR	20.0593
θ MOGPR	20.0594


Synthetic dataset, predicted profile and test profile
Temperature (K)
300
400
500
600
700
0
20
40
60
80
100
Path lenght (cm)
Predicted value
Test profile


Predicted temperature profile
Experimental test point
Experimental case predicted profile and experimetal data point
Temperature (K)
700
650
600
550
500
450
400
350
300
0
20
40
60
80
100
Path lenght (cm)

Observations

In the simulated dataset:

- The β MOGPR (LMC + AWGN noise) model exhibited the best testing loss.
- Following closely was the β MOGPR (ICM + AWGN noise) model.
- Noise-modeled models outperformed noise-free trained models, suggesting noise modeling enhances prediction accuracy.

Observations on ICM and LMC models:

- ICM models demonstrate consistency across datasets, beneficial for stability.
- LMC models achieve higher accuracy with some variability, advantageous for maximizing predictive performance.

Real-world test case findings:

- All models showed similar error values in the real-world test case.
- Convergence of error values across different modeling approaches in practical settings highlights complexities and uncertainties.
- Emphasizes the importance of adapting modeling strategies for real-world data variability and unpredictability.

Conclusions

LMC vs. ICM Sampling:

- LMC samples from different GPs, fitting data better but sensitive to data and noise.
- ICM samples from one GP, consistent across datasets, and resilient to noise.

Factors Impacting Experimental Testing:

- **Modeling of the Real-World Temperature Profile**: Crucial for accurate representation of the environment.
- **Noise Modeling in Simulated Data**: Understanding and accounting for noise is essential.
- **Effect of External Interference**: Consideration of external factors impacting experimental results.

- **Change in Mole Fraction (X)**: Monitoring X changes and its impact on the system.
- **Amount of Synthetic Samples Used**: Influences robustness and generalizability of results.
- **Low Quantity of Experimental Data**: Limitations in insights gained, importance of collecting more data.

Note:

- Experimental test conducted on a single set of data, limiting conclusive insights.
- Testing on a broader range of real-world datasets would enhance understanding and conclusions.

Future Scope and improvements

- **Specialized Kernel**: Optimize model performance by tailoring kernel choice to problem specifics for improved accuracy.
- **Large Synthetic Dataset**: Enhance model robustness with an extensive dataset to capture diverse patterns and variations effectively.
- **Improved Noise Modeling**: Boost accuracy and generalization by refining noise representation to better reflect data uncertainties.
- **Experimental Data Usage**: Improve model fidelity by integrating real data to capture real-world complexities comprehensively.
- **Deep Learning Techniques**: Utilize neural networks for sophisticated modeling of intricate data relationships and high-dimensional data effectively.

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The End

Questions? Comments?