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ScienceDirect

Energy Procedia 129 (2017) 915–922

Energy Procedia

www.elsevier.com/locate/procedia

IV International Seminar on ORC Power Systems, ORC2017
13-15 September 2017, Milano, Italy

Evaluating the quality of steady-state multivariate experimental data relative to various ORC experimental setups

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Abstract

Today, an increasing amount of experimental data is being released in the ORC field. This data is required to assess and compare the performance of different machines, to point out the main sources of losses, or to calibrate and to validate models.

Experimental data is subject to different sources of disturbance and errors whose importance should be assessed. The level of noise, the presence of outliers, or a measure of the "explainability" of the key variables with respect to the externally imposed operating condition are important indicators, but are not straightforward to obtain, especially if the data is sparse and multivariate.

Starting from recent experimental campaigns on two different ORC test rigs, this paper proposes a methodology and a suite of tools implementing Gaussian Processes for quality assessment of steady-state experimental data. The aim of the proposed tool is to (1) provide a smooth (de-noised) multivariate operating map of the measured variable with respect to the inputs; (2) determine which inputs are relevant to predict a selected output; (3) provide a sensitivity analysis of the measured variables with respect to the inputs; (4) provide a measure of the accuracy (confidence intervals) for the prediction of the data; (5) detect the observation that are likely to be outliers.

In this paper, the ORC test rigs and the obtained experimental data are described. The results are then analysed with the proposed tool, and compared with the results of traditional modelling techniques. It is demonstrated that GP regression provides insightful numerical indicators for these purposes, and that the obtained performance is higher or comparable to alternative modelling techniques. Finally, the datasets and tools developed in this work are provided within the GPexp open-source package.

Peer-review under responsibility of the scientific committee of the IV International Seminar on ORC Power Systems.

Keywords: Gaussian Processes; Kriging; Experimental; Outliers; Feature selection; Organic Rankine Cycle; ORC

1. Introduction

An increasing amount of experimental data is being released in the ORC field. This data is required to assess and compare the performance of different machines, to point out the main sources of losses, or to calibrate and to validate models.

However, this experimental data is subject to many sources of noise and errors, such as sensor malfunctions, transient phenomena, operator misuse of the test rig, noise in the data acquisition chain, unaccounted for external

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Peer-review under responsibility of the scientific committee of the IV International Seminar on ORC Power Systems.
10.1016/j.egypro.2017.09.107

influences, etc. It is therefore of primary importance to assess the its quality, by evaluating the level of noise, the presence of outliers, or to measure the explainability of the acquired variables with respect to the externally imposed operating condition. This task is far from straightforward, especially if the data is sparse and multivariate.

Gaussian Processes (GP) are an active field of research in machine learning and provide a powerful tool for the above purposes. Their Bayesian formulation allows predicting the variable of interest for new/unseen data points and provides coherent estimates of predictive uncertainty. The method reduces predictive confidence when extrapolating away from the data points: if the data density is locally high, the variance is small, on the opposite, if the density is low, the variance is larger, leading to more distant confidence boundaries. Furthermore, the method is highly flexible and can accommodate a range of covariance structures - including non-linear relationships - and delivers state of the art prediction performance

In this work, we use GPExp, a library developed at the University of Liege, to evaluate experimental data in a GP framework. The main features of the tool are the following:

1. Provide a smooth (de-noised) multivariate operating map of the measured variable w.r. to the inputs.
2. Determine which inputs are relevant to predict a selected output (feature selection)
3. Provide a sensitivity analysis of the output with respect to the inputs
4. Provide the accuracy (confidence intervals) to predict the output with a given set of inputs. This interval should be function of the data density.
5. Detect the observation that are likely to be outliers

This paper presents the development of the tool and illustrates, through examples, how it can be used to detect the main dependencies, shortcomings and outliers in experimental data. Examples are first described for univariate or bivariate processes, whose quality can be assessed visually, and then extended to real ORC processes with multiple input variables. The experimental data relative to three different test rigs is compared.

The tool is developed in such a way that a qualitative interpretation of the results is provided to users who are not specialist in machine learning. It comprises a Graphical User Interface (GUI) and can be freely downloaded and tested.

2. Gaussian Processes as a data analysis tool

2.1. Gaussian Processes Regressions

This section provides a brief explanation of Gaussian Processes regression. The interested reader can refer to [1] for a more detailed description.

When performing a regression, the goal is to find a function f that maps each input x to the variable of interest, a.k.a. target y. The type of function f is usually set *a priori* by the user. Furthermore, hyperparameters, such as the order of a polynomial fit, also need to be fixed *a priori*. Increasing the complexity of f can in most cases lead to an excellent fit of the data. However, too complex models also fit the noise in the data (i.e. they ”over-fit”), which is not desirable [2].

Gaussian Processes, on the contrary, are based on the Bayesian analysis of the standard linear model:

$$f(\boldsymbol{x}) = \boldsymbol{x}^T \boldsymbol{w} \tag{1}$$

$$\boldsymbol{y} = f(\boldsymbol{x}) + \boldsymbol{\varepsilon} \tag{2}$$

with $\boldsymbol{w} \in R^m$, the vector of parameters (weights) of the model and $\boldsymbol{\varepsilon}$ an error term distributed according to a Gaussian distribution with zero mean and variance σ_n^2.

Let $X \in R^{n\times m}$ be the matrix concatenating all n data points and $\boldsymbol{y} \in R^n$ be their corresponding targets. Bayes' rule allows computing the probability density of the observations given the model parameters $p(\boldsymbol{y}|X, \boldsymbol{w})$, a.k.a. the likelihood and infer on the model parameters:

$$p(\boldsymbol{w}|\boldsymbol{y}, X) = \frac{p(\boldsymbol{y}|X, \boldsymbol{w})p(\boldsymbol{w})}{p(\boldsymbol{y}|X)} \tag{3}$$

Finally, the predictive distribution of a new/unseen sample x^* can be estimated from $p(f^*|x^*, X, \boldsymbol{y})$, which is also Gaussian, allowing to make predictions.

In the Gaussian Processes approach, the priors are defined over the function f instead of on the model parameters $\boldsymbol{w}$ (this is referred to as the "function space"). f is assumed to follow a Gaussian Process, i.e. a multivariate Gaussian distribution:

$$f(\boldsymbol{x}) \sim N(\mu(\boldsymbol{x}), k(\boldsymbol{x}, \boldsymbol{x}')) \tag{4}$$

with $\mu(\boldsymbol{x})$, the mean latent function and $k(\boldsymbol{x}, \boldsymbol{x}')$, the covariance function, or kernel.

This formulation highlights the central role of the kernel, which defines the distribution over functions. The kernel is chosen as an Automatic Relevance Determination [3] kernel. This kernel is a squared exponential kernel with a distinct parameter l defined for each variable d=1...D. This hyperparameter represents the "length-scale" of the kernel in each direction. In the ARD kernel, if a length-scale is large, a long distance needs to be travelled before seeing significant changes in the corresponding direction. Therefore, the corresponding variable does not have much influence on the model.

$$k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sigma_f^2 \cdot exp(-\frac{(\boldsymbol{x}_i - \boldsymbol{x}_j)^2}{2 \cdot l_i^2}) \tag{5}$$

The hyperparameters σ_f and l_i are optimized based on the marginal likelihood $p(\boldsymbol{y}|X)$ (Eq. 3), which takes into account both the goodness-of-fit and the complexity of the model.

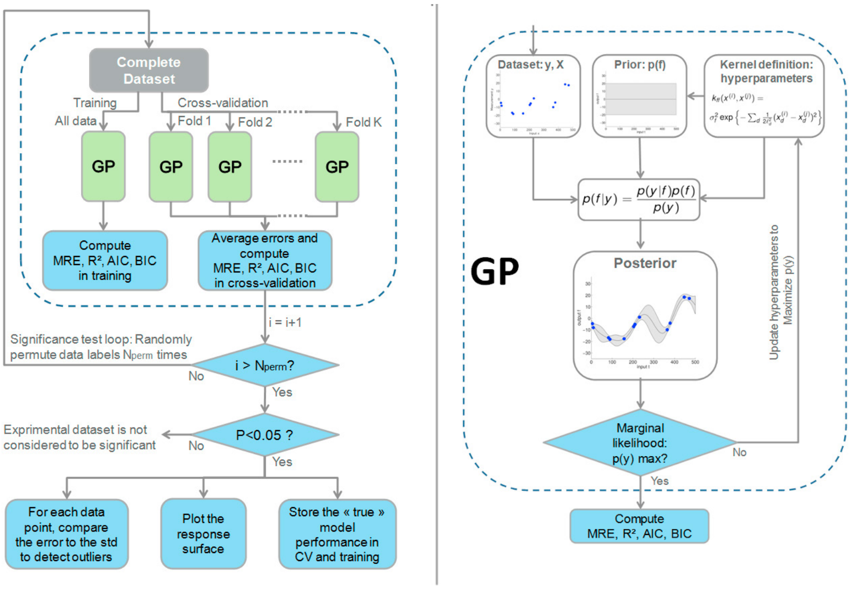

Fig. 1. Schematic view of the analysis

3. Experimental Setups

3.1. Reversible Heat Pump / ORC unit

This section presents an experimental campaign carried out on an innovative reversible heat pump (HP) / organic Rankine cycle (ORC) unit. The concept of a reversible HP/ORC system integrated into a residential building with a solar roof is described in [4]. The following focuses on the layout and a complete description of the components and sensors of the test-rig.

A scheme of the test rig is provided in Figure 2 with the main elements shown; compressor, evaporator, condenser, pump and valves. The refrigerant loop (dark blue) also includes a liquid receiver for charge variations and a sub-cooler used to provide a sufficient degree of sub-cooling at the inlet of the pump. This loop also includes a four-way valve that allows for switching between ORC and HP modes and a bypass valve that is necessary to start the expander in ORC mode. The evaporator is supplied by a water loop (red) connected to an electrical boiler (150 kW). The condenser is cooled by tap water (light blue) to simulate the cold water flow in the storage or the ground heat exchanger, depending on the mode of operation.

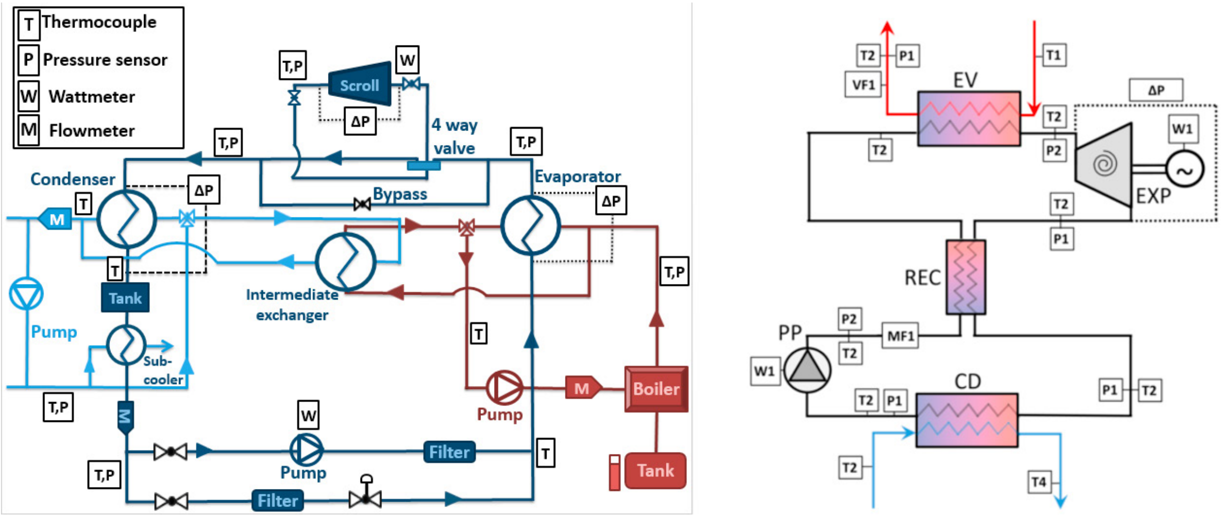

Fig. 2. Detailed scheme of the HP/ORC setup (left) and of the Sun2Power setup (right)

The compressor has been modified following the methodology proposed by Quoilin [5] to allow its operation as an expander or as a compressor. These modifications include the opening of the casing, the removal of the check valve and the addition of a spring below the floating seal. Plate-type heat exchangers are used for the evaporator and condenser. They are selected for their compactness, efficiency and low cost. The pump is a volumetric plunger-type pump whose rotational speed is controlled by an inverter. An electronic expansion valve is chosen for its controllability compared to traditional expansion valves. Detailed characteristics of the setup can be obtained in [4].

Measurements are performed in steady-state conditions and averaged on a five minutes basis. Table 1 presents the variation range of the main operating conditions observed in both modes for the stabilized measurement points [4].

Table 1. Experimental results for the HP/ORC unit

	ORC		Heat Pump	
	Minimum	Maximum	Minimum	Maximum
Evaporator/condenser thermal power [kW]	30	65	9	17
Evaporation pressure [bar]	16	32	3	6.5
Condensation pressure [bar]	5.4	10.2	6	20.5
Mass flow rate [kg/s]	0.124	0.294	0.049	0.113
Expander/compressor electrical power [kW]	0.125	3.696	1.87	4.3
Overall efficiency / COP [-]	0	0.053	2.7	7.1
Expander/compressor isentropic efficiency [%]	10	63	69	79
Expander/compressor volumetric efficiency [-]	1	1.1	0.95	1.15

3.2. Low capacity solar ORC

This system is referred to as the Sun2Power ORC module and is developed at the University of Liege [6,7]. It is a 3 kWe recuperative organic Rankine cycle using R245fa as working fluid. It is constituted of a scroll expander with variable rotational speed and a diaphragm pump. Both the recuperator and the evaporator are brazed plate heat exchangers (protected with a 3 cm-thick thermal insulation), while an air-cooled fin coil heat exchanger is used for the condenser. Variable-frequency drives are used to control both the rotational speeds of the pump and the condenser fan. On the other hand, the expander rotational speed is controlled by means of a variable electrical load. A schematic view of the system is proposed in Figure 2. Although not indicated, rotational speeds for the pump, the expander and the condenser fans are also monitored.

3.3. Open-drive scroll expander

The third experimental campaign focuses on the expansion machine only (a scroll expander). The results of the experimental campaign were published in [8], together with a comprehensive description of the test rig. In that setup (Figure 3) the input values ”imposed” to the scroll expander were the working fluid flow rate $\dot{M}$, the rotational speed N_{rot}, the supply temperature T_{su}, the exhaust pressure p_{ex} and the ambient temperature T_{amb}. The measured outputs were the supply pressure p_{su}, the exhaust temperature T_{ex} and the output shaft power $\dot{W}_{sh}$. It should be noted that there is no firm causality relationship between these variables, except for T_{ex} (which is always an output) and T_{amb}, which is always an input. All the other variables can independently be inputs or outputs of the model. As an example, if p_{su} is imposed in the test rig instead of $\dot{M}$, the flow rate is imposed by the expander and becomes an output. In total, there are always 5 different inputs, the other variables being consequences of the scroll expander performance and therefore outputs of the model.

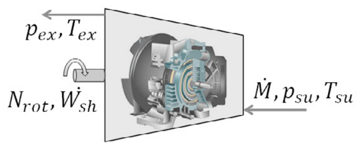

Fig. 3. View of the tested scroll expander with the measured variables

In [5], the authors of the study developed a semi-empirical model of the machine. This kind of model accounts for most of physical phenomena and losses in the machine, but requires experimental data for their calibration. A total of 36 data points were used to tune the 6 empirical parameters of the model. A comparison between the model prediction and the measurement was performed, but without cross-validation. The obtained MAE was 1.94% and the R^2 value was 98.81%.

3.4. Summary

Each considered system is characterized by measured inputs variables (or features) and measured output variables. One of the goal of this analysis is to evaluate the ”explainabilty” of each output with respect to the inputs. To that end, one single output, the expander power. is selected for the three test rigs. The two ORC systems are seen as black boxes, i.e. their inputs are secondary fluids (heat source and sink) and the user-defined set points (e.g. the pump speed). In the case of the expander, the exogenous inputs are the inlet and outlet conditions and the ambient temperature, as described in section 3.3. These different variables are summarized in Table 2.

Table 2. Inputs variables of the three considered processes

HP/ORC		Sun2Power		Expander	
Heat source flow rate:	$\dot{M}_{su,ev}[kg/s]$	Heat source flow rate:	$\dot{V}_{su,ev}[kg/s]$	Inlet pressure:	$P_{su}[Pa]$
Heat sink flow rate:	$\dot{M}_{sf,cd}[kg/s]$	Heat sink flow rate:	$\dot{V}_{sf,cd}[kg/s]$	Outlet pressure:	$P_{ex}[Pa]$
Heat source temperature	$T_{hf,su,ev}[K]$	Heat source temperature	$T_{hf,su,ev}[K]$	Rotating speed:	$N_{rot}[rpm]$
Heat sink temperature	$T_{cf,su,cd}[K]$	Heat sink temperature	$T_{cf,su,cd}[K]$	Inlet temperature:	$T_{su}[K]$
Pump speed:	$N_{pp}[rpm]$	Expander Rotating speed:	$Hz_{pp}[s^{-1}]$	Ambient temperature:	$T_{amb}[K]$
		Expander Rotating speed:	$Hz_{exp}[s^{-1}]$		
		Condenser fan speed:	$Hz_{cd}[s^{-1}]$		
		Ambient temperature:	$T_{amb}[K]$		

4. Gaussian Processes analysis

In this section, an ex-post evaluation of the experimental results presented above is performed. The same dataset has been used and tested in GPExp, using the methodology described above. Examples of Gaussian Processes regressions are presented in Figure 4, predicting the expander isentropic efficiency with one or two input variables. In the univariate case, the error in cross-validation is 5.9% and the standard deviation is relatively high, whereas in the bi-variate case, the average error is reduced to 5.3%. This new input is therefore considered as relevant.

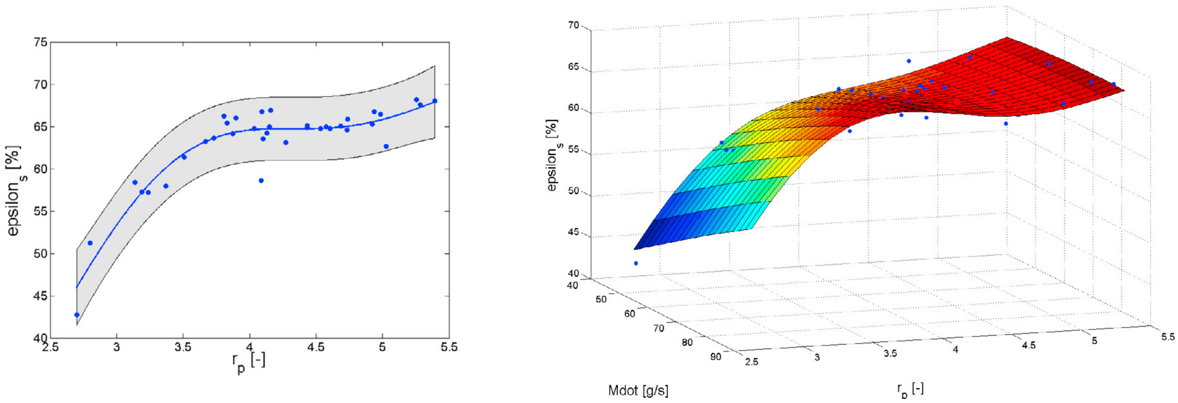

Fig. 4. GP regression of the expander efficiency as a function of one input (left) or two inputs (right)

4.1. Outlier detection

Some data points can have target values that do not represent the underlying latent function. Such situations can arise e.g. in case of sensor malfunction, or if the output was impacted by a phenomenon that is not accounted for in the inputs. These points can be considered as outliers, and might have to be removed from any further analysis.

Gaussian Processes have proven to be a powerful framework to detect outliers (see e.g. [9]) since the variance of the GP regression function varies with the data density and with the noise, as shown in the previous section. The effect of outliers is illustrated in Figure 5 for the case of the HP/ORC test rig: two data samples clearly present a high error compared to smooth GP response surface. They are therefore most likely outliers. In the case of a normal distribution, a significance level lower than 5 percent corresponds to an error higher than 1.96 times the standard distribution. This threshold is the one selected in this work.

Figure 5 shows that, according to this threshold data points 11 and 14 can be considered as outliers in the HP/ORC experimental results. An additional unaccounted for input explaining their deviation should therefore be added to the analysis. In case no external effect can be found, the data should be checked carefully for any mistake or malfunction, and the two points might be removed from the analysis.

4.2. Sensitivity analysis and feature detection

In case of multivariate processes, it is important to evaluate the variables influencing significantly the output and discard those that are not necessary to the model. This task is complex, especially in the case of high dimension non linear systems.

The Sun2Power test rig is selected for the present analysis, because it is the process that possesses the highes number of input variables. The goal is therefore to select the relevant variables among them (feature selection) and evaluate their sensitivity.

Feature selection is performed by iterative block addition, as proposed in [10]: if adding a new input decreases the MAE in cross-validation, the input is considered relevant. Otherwise, this additional variable only adds noise by increasing the complexity of the model without contributing to the prediction of new/unseen data samples. It can therefore be disregarded.

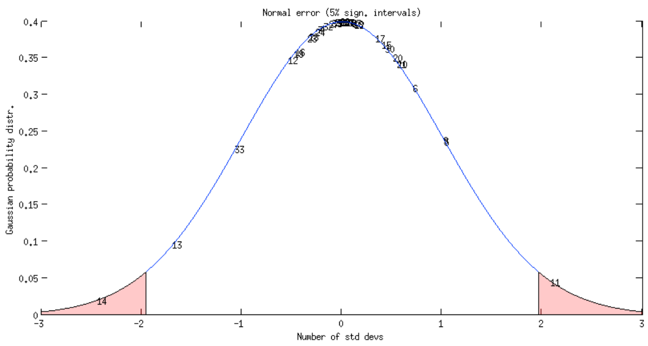

Fig. 5. Distance between each data point and the GP regression for outlier detection

The results of the analysis are presented in Table 3 for a "leave-one-out" cross-validation. As expected, the MAE for the whole training set is higher than the MAE in cross-validation for all combinations of input, but the difference remains limited (lower than a factor two in this case). This indicates that the model is most likely not overfitting. It can also be noted that the MAE in cross-validation keeps decreasing when adding inputs to the model, except for T_{amb}, $\dot{V}_{su,ev}$ and $T_{cf,su,cd}$. These variables should therefore not be taken into account for the prediction of the output power since don't have a significant impact in this dataset and would only bring random variations to the model.

Finally, the implementation of the automatic relevance determination (ARD) kernel [3] allows evaluating the sensitivity of the output to different inputs. Large lengthscales prohibit fast variations of the GP function in the direction of the respective input. In Table 3, the optimal lengthscale for each input is provided in the case of the optimization with all variables. It is worthwhile to note that the irrelevant variable described above are characterized by high lengthscales, which is therefore another manner to perform feature selection. Furthermore, the lengthscales of the relevant features provide a measure of the sensitivity of this input with respect to the output (the lower the lengthcale, the higher the sensitivity).

Table 3. Effect of the selected input variables on the MAPE and lengthscales associated with these variables

Input variables	Removed variable	Lengthscale	MAPE (full dataset)	MAPE (cross-validation)
$\dot{V}_{su,ev}$ $\dot{V}_{sf,cd}$ $T_{hf,su,ev}$ $T_{cf,su,cd}$ Hz_{pp} Hz_{exp} Hz_{cd} T_{amb}	T_{amb}	27.3	0.0055	0.0535
$\dot{V}_{su,ev}$ $\dot{V}_{sf,cd}$ $T_{hf,su,ev}$ $T_{cf,su,cd}$ Hz_{pp} Hz_{exp} Hz_{cd}	$\dot{V}_{su,ev}$	528	0.0055	0.0492
$\dot{V}_{sf,cd}$ $T_{hf,su,ev}$ $T_{cf,su,cd}$ Hz_{pp} Hz_{exp} Hz_{cd}	$T_{cf,su,cd}$	27.3	0.0055	0.0491
$\dot{V}_{sf,cd}$ $T_{hf,su,ev}$ Hz_{pp} Hz_{exp} Hz_{cd}	$\dot{V}_{sf,cd}$	11.5	0.0051	0.0473
$T_{hf,su,ev}$ Hz_{pp} Hz_{exp} Hz_{cd}	$T_{hf,su,ev}$	1.95	0.0051	0.0456
Hz_{pp} Hz_{exp} Hz_{cd}	Hz_{exp}	1.15	0.0243	0.0557
Hz_{pp} Hz_{cd}	Hz_{pp}	1.31	0.0631	0.0864
Hz_{cd}	Hz_{cd}	0.32	0.1749	0.1978

4.3. *Overall quality of the datasets*

The overall quality of the data can be evaluated by measuring the average distance of the measurement with the smooth GP regression (considered to be the ideal model). This quantity provides a benchmark for other types of models applied to this data: if their error is significantly higher it indicates a margin for improvement. If it is smaller, the proposed model is most likely overfitting and should be corrected.

For the three experimental datasets used in this work, a physical model was previously proposed and calibrated with the data. The results of these models can therefore be analysed *ex post* and compared to the outputs of the GP regression. This is performed in Table 4.

Table 4. Mean average percentage error obtained with the GP regression and with the physical models

Dataset	GP regression	Physical model
HP/ORC	1.92%	2.45%
Sun2Power	4.56%	8.12%
Expander	0.998%	1.94%

5. Conclusions

This paper presents a methodology to analyse experimental steady-state data. The method relies on Gaussian Processes regression, which is a well known technique, but had, to our knowledge, never been applied to the critical analysis of monitoring data.

Data quality is evaluated using numerical model performance indicators by comparing it to the GP regression latent function. These indicators are useful, e.g. to assess the quality of the correlation between some measured operating conditions (inputs) and some measured performance data (outputs). They also set a benchmarking standard to compare different sets of experimental data. Furthermore, the probabilistic formulation of Gaussian Processes provides confidence intervals to predict the output with a given set of inputs, which are a function of the noise and of the local data density.

In addition to the evaluation of the data quality, the method also helps evaluating which variables are relevant to the selected model. The feature selection capability allows determining the relevant inputs for the prediction of one output variable. In this paper, this is achieved by means of two different but converging techniques: the comparison of the cross-validation errors with recursive feature addition, and the comparison of the lengthscales relative to each input.

It is further demonstrated, through examples, how the proposed tool can efficiently be used to detect the main dependencies, shortcomings and outliers in experimental data. Examples are first described for the univariate case, whose quality can be assessed visually, and then extended to processes with multiple input variables.

The method is implemented within the open-source tool GPexp to ensure a good transparency and reproducibility of the work [11]. It is developed in such a way that a qualitative interpretation of the results is provided to users without machine learning expertise. It comprises a Graphical User Interface (GUI) and can be freely downloaded and tested.

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