DATA ASSIMILATION FOR FUEL PERFORMANCE CODE DEVELOPMENT: APPLICATION TO OXIDE FUEL THERMAL PROPERTIES

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ABSTRACT

Data assimilation methods are suitable tools for handling experimental data and extracting synthetic results from them. In this work, the Gaussian Process (GP) method for making regressions on the thermal properties of fuel is presented. GP is a nonparametric supervised learning method used to solve regression and probabilistic classification problems. A GP regression model can make predictions incorporating prior knowledge (kernels) and provide uncertainty measures over predictions, with the advantage of not requiring assumptions about the shape of the correlation but relying only on the data set. The objective is to demonstrate the validity of this approach for choosing thermal property values within Fuel Performance Codes (FPCs) for the fuel pin thermo-mechanical analysis, for which two test cases are shown: melting temperature and thermal conductivity. For this purpose, experimental data regarding the MOX fuel are treated with Gaussian processes and the obtained synthetic results are provided to the TRANSURANUS FPC, without increasing the computational demand while running the FPC. These models were implemented as an external shell written in the Python language for SCIANTIX, an open-source meso-scale code to describe inert gas behaviour in nuclear fuel, that can be coupled with FPCs. The implementation is performed in a modular flexible way, to be extended to full set of models and properties.

1. Introduction

FPCs are essential tools for simulating the behaviour of nuclear fuel pins under various operating conditions. These codes rely on accurate quantities, such as material properties or model parameters, to solve physical models effectively. For instance, in performing thermo-mechanical analysis, FPCs like TRANSURANUS [1] or OFFBEAT [2] require material properties.

Typically, the followed approach is based on obtaining empirical or semi-empirical correlations from experimental data, which are then input into the algorithm [3]. Recently, efforts have been made to simplify this process by using machine learning approaches to complement more traditional methods based on statistical data analysis [4].

In this work, we apply a data-driven method to update the semi-empirical correlations describing fuel melting temperature and fuel thermal conductivity, with available experimental data. The method is the GP [5], a probabilistic supervised machine learning framework that has been widely used for regression and classification tasks. The goal of the tool is to handle the experimental data on its own, giving the reference code the correlation trend without needing external evaluation or assumption on the shape of the correlation.

1.1. Method

Gaussian process is a classical machine learning method to handle regression/classification problems (this distinction relies on the continuity/discrete nature of the problem). It is a stochastic process, namely a collection of random variables, such that every finite collection of those random variables has a multivariate normal distribution. The distribution of a Gaussian process is the joint distribution of all those (infinitely many) random variables, and as such, it is a distribution over functions with a continuous domain that can be fully specified by its mean function $\mu(x) = \mathrm{E}[Y(x)]$ and its covariance function $C(x, x') = \mathrm{E}\big[\big(Y(x) - \mu(x)\big)\big(Y(x') - \mu(X')\big)\big]$ [6]. In our case, X will be the input space with a dimension equal to the number of inputs, x is the independent variable and Y (x) is the random variable. The kernel adopted for regression may be specified in the tool and, in this case, it is a constant kernel multiplied by the standard Radial basis function (RBF) kernel, defined as:

$$K(x, x') = \sigma \exp\left(-\frac{|x - x'|^2}{2l^2}\right)$$

Where K is the defined kernel and, σ and l are the two hyperparameters required as input. The first one describes how much vertically the function can span, the second one, instead, represents how quickly the correlation relationship between two points drops as their distance increases. The method has been implemented as an external Python shell in the SCIANTIX codeFare clic qui per immettere testo., in a way that allows for two types of approaches:

- Direct fit of the experimental points
- Update the correlation taken as a reference, based on a fit of the distances between it and the experimental points considered

In addition, since the method returns a matrix of values on the grid provided for kernel evaluation, a multilinear interpolator is implemented to compute predictions given a certain input.

The effectiveness of the data regression, beyond the graphical display of the result, can be evaluated through indicators, such as the logarithm marginal likelihood, that if higher suggests a better fit of the model to the data, and the mean square error, to be compared with the equivalent values of other regression methods. Also, predictive posterior checks can be performed: by generating synthetic data from the posterior predictive distribution and comparing them with the observed data.

1.2. Quantities of interest

To show the capabilities of the developed tool, two properties are taken into consideration:

- MOX fuel melting temperature, as a function of plutonium content and stoichiometry deviation
- Nuclear fuel thermal conductivity, as a function of temperature, plutonium content, americium content, stoichiometry deviation and porosity

The correlations used to perform the update are taken from the work by Magni et al. [3], then, as a comparison, the correlation for the fuel melting temperature from the work by Di Gennaro et al. [9] is plotted against the results obtained in this work.

2. Results

As first analysis, we consider the results obtained on the MOX fuel melting temperature considering it only as a function of the plutonium content. In Figure 2.1 it is possible to see the comparison between the direct fit on the whole dataset and the update performed from the correlation from the work of Magni et al. [3]. It should be noted that, in this case, the update criterion was made to vary with plutonium content, since the correlation has a limit of validity for a plutonium content value of 45 %, consequently, as one moves away from the threshold, the method performs a fit over an increasing fraction of the distance between the experimental data and the correlation. The quadratic fit from the work of Di Gennaro et al. [9] is also presented, as a comparison. The logarithmic marginal likelihood of the GP regression is 117.

Considering now the complete case, namely, the melting temperature as a function of the plutonium content and the stoichiometry deviation, results are shown in Figure 2.2 and Figure 2.3. The vertical distance between the correlation and the experimental data is fitted to obtain a distance function, then, a fraction of it could be added to the old correlation to obtain the updated one. As a first attempt, a value of 0.5 was selected, which can be changed depending on how reliable we consider the experimental data to be in relation to the starting correlation. The final prediction is thus obtained through:

$$T_{melt} = T_{melt,\,old} + \alpha \cdot d_{GP}$$

Where $T_{melt,\,old}$ is the MOX melting temperature predicted by the correlation by Magni, α is a weight factor and d_{GP} is the value of the distance function.

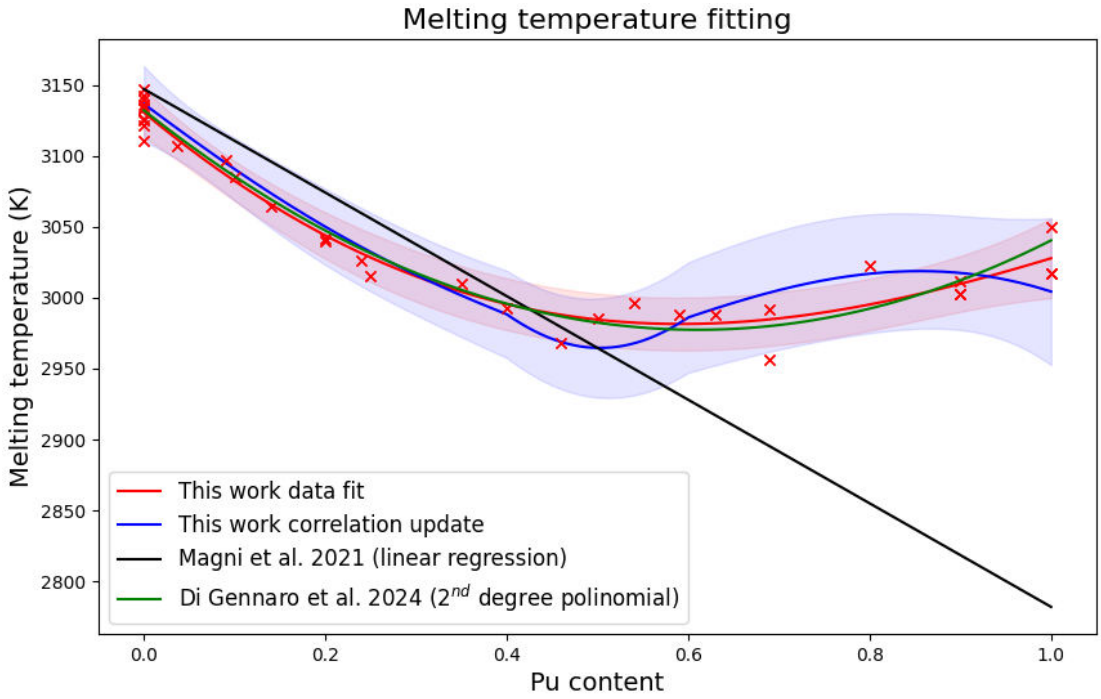

Figure 2.1: Comparison of MOX melting temperature data fitting and correlation update against linear regression from the work by Magni et al. [3] **and the quadratic regression from the work by Di Gennaro et al.** [9]**.**

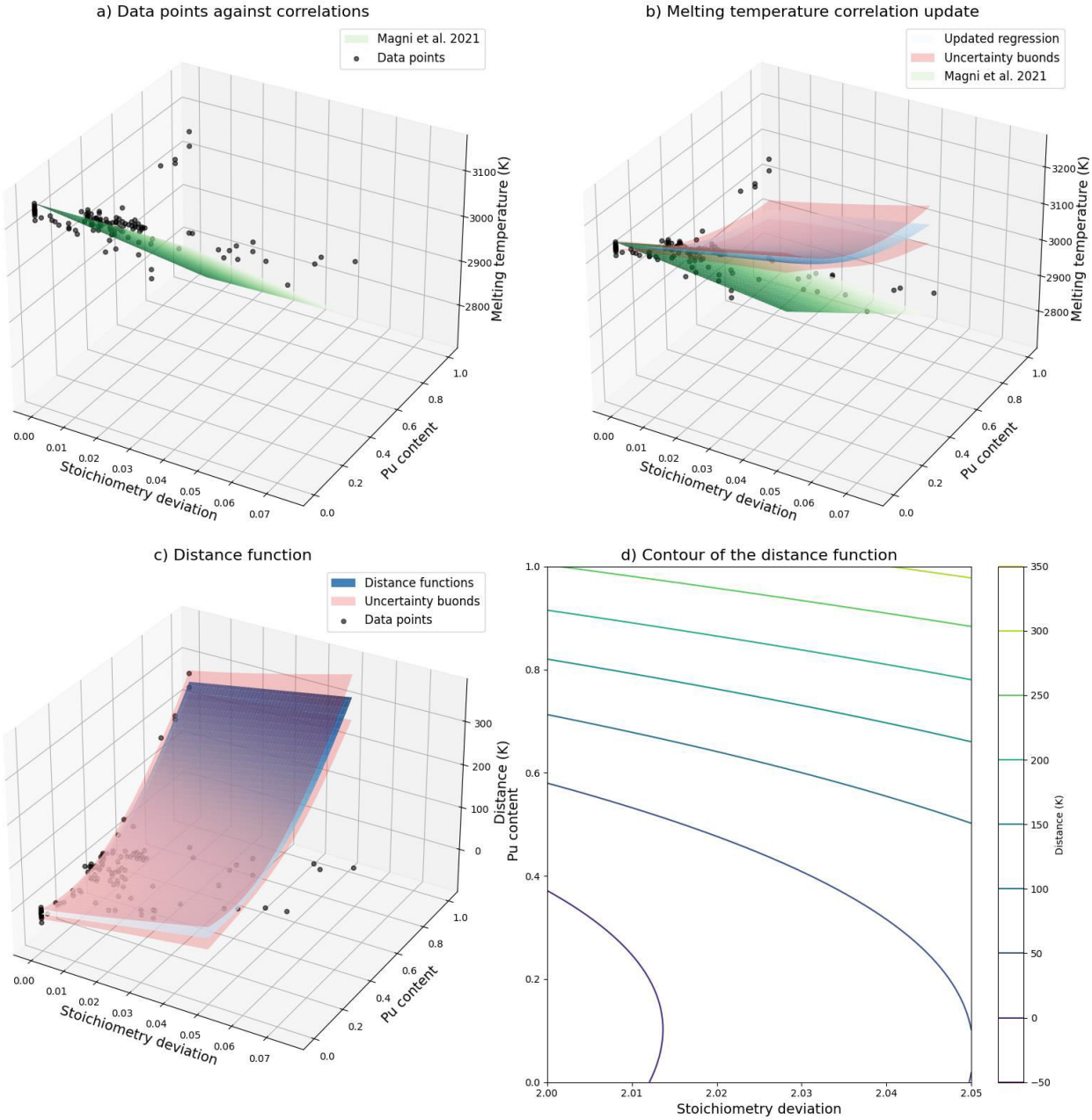

Figure 2.2: Melting Temperature data plotted against the correlation by Magni [3] **(a), the updated correlation against the old one (b), the distance function, obtained by fitting distances between data and correlation surface, with its uncertainty (c) and a contour plot of the distance function (d). Note that, in this case, half of the weight function is added to the correlation to obtain the new prediction.**

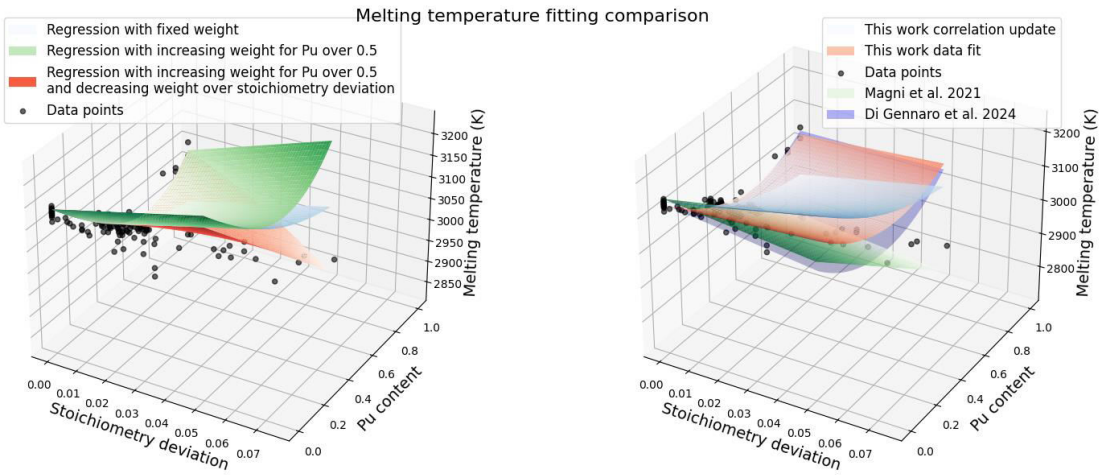

Figure 2.3: Comparison between the melting temperature correlation update considering a fixed weight (0.5), a weight that is progressively increasing after the validity threshold of the correlation by Magni [3], namely a Plutonium content equal to 45%, and a weight that, in addition, is decreasing with the increasing of the stoichiometry deviation, on the left, and comparison between the correlation, in green, the one by Di Gennaro [9], in violet, the fit of the whole dataset with GPs, in red, and the update of the correlation by Magni with GPs, in blue, on the right.

Regarding the thermal conductivity of fuel, it is necessary to introduce the concept of local evaluation. In fact, being a function of five variables, evaluating the regression kernel on a dense grid is impossible because of the size of the vector. Therefore, it is convenient to perform an evaluation in a neighbourhood of the selected irradiation history, choosing whether to consider all experimental points or only those close to the selected history.

In addition, given the impossibility of graphically visualizing the regression, two hypothetical irradiation histories are shown in Figure 2.4, suitable for representing fictitious situations to evaluate the effectiveness of the thermal conductivity assessment. Figure 2.5 shows the predictions with respect to the regression from the work by Magni et al. [3], highlighting the experimental points close to the conditions chosen for the five variables. Finally, Table 1.1 shows the summary parameters that can be used to compare the quality of the regression performed with GPs against those obtained with traditional statistical methods.

Table 1.1: Regression parameters for the GP regression and the correlation by Magni et al. [3]

Regression	Logarithmic marginal likelihood	Mean square error (MSE)	Coefficient of determination (R^2)
GP fit	217	0.018	0.93
GP update	242	0.028	0.6
Magni's correlation	-	0.01	-

In the first history, temperature ramps are simulated to show how this is the most impactful variable in the calculation of thermal conductivity. In this case, updating the correlation tends to correct it upward because the experimental data tend to be greater than the values predicted by the correlation. In the second case, we consider a constant temperature and a high plutonium content. It can be observed that, in the absence of nearby experimental points, the correlation is not actually updated.

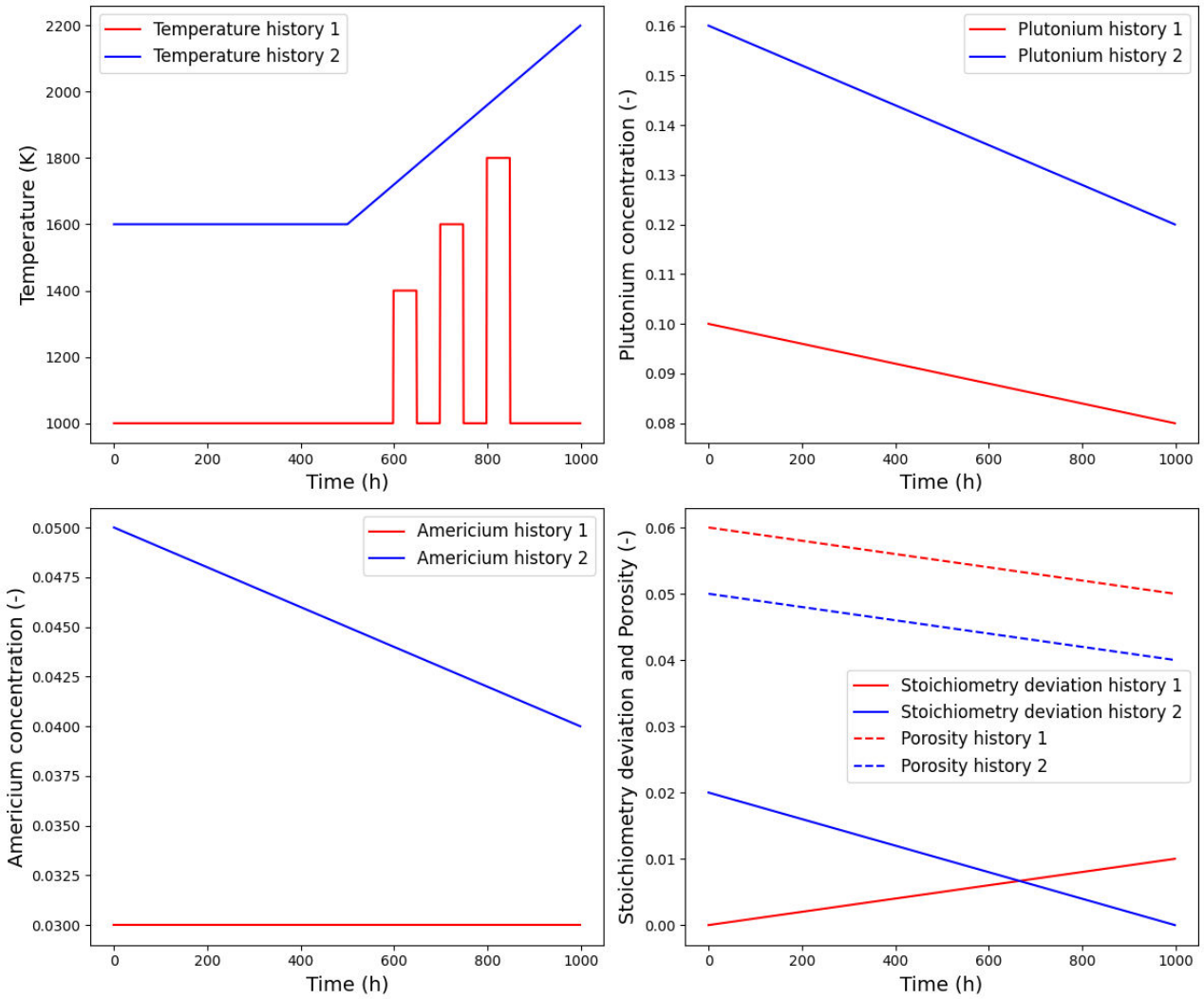

Figure 2.4: Fictitious irradiation histories, showing a hypothetic evolution of temperature, plutonium content, Americium content, Stoichiometry deviation and porosity over time.

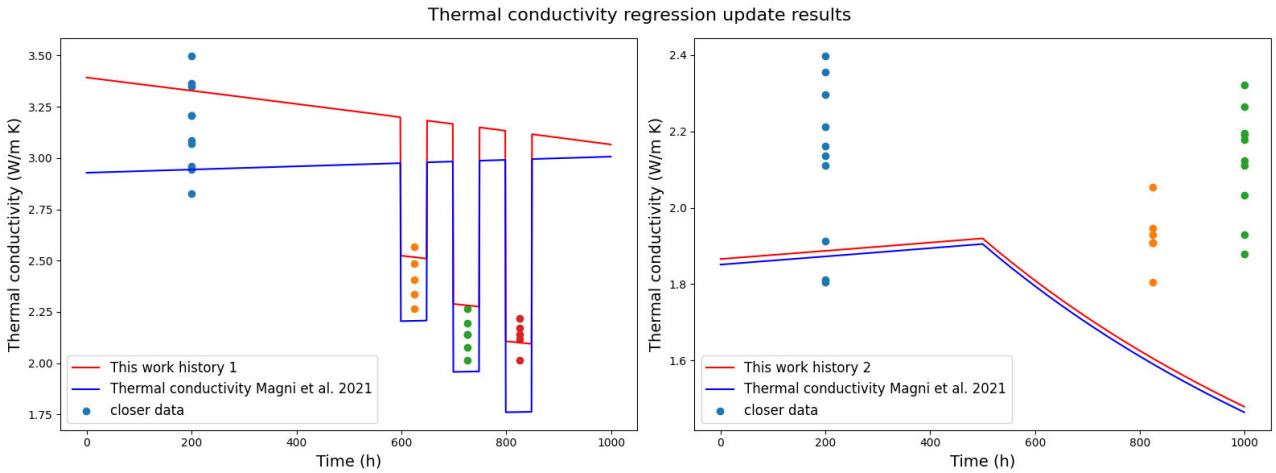

Figure 2.5: Thermal conductivity obtained in this work, in red, against the one calculated with the correlation by Magni [3], in blue. In addition, the closest experimental values, are represented for different times in the fictitious histories.

3. Discussion

Regarding the one-dimensional case, with the melting temperature only function of plutonium content, good results are observed and, in general, the method performs well in these situations downstream of minimal data preprocessing. The only aspect to be taken into consideration has to do with the validity range of the previous correlation, beyond which greater importance is given to the new experimental points. Whereas, in the two-dimensional case the way we decide to update the correlation turns out to be decisive. The overall best performance is obtained with the pure GP fit, while, if the aim is to correctly reproduce the high stoichiometry deviation-high plutonium region, the best result is obtained by updating the correlation by adding to it a fraction of the distance function that decreases with increasing plutonium content and with deviation from stoichiometry. This case is shown in detail in Figure 3.1.

The approach followed is to weight the fitting of the distances between the correlation and the experimental points, by an appropriate trust function that is related to the uncertainty of the points and their distance from the correlation. In this way it is possible to make a correction that, for close points, lies somewhere between them and the correlation, and as one moves further away from the correlation more weight is given to the experimental points, if they are reliable.

The predicted values against the experimental ones and the residuals are shown in Figure 3.2 and 3.3. It can be seen that the pure GP fit exhibits the best overall performances, even if it tends to underestimate the MOX melting temperature. While, with the update settings it is possible to be more conservative in this sense, despite the highest residuals.

As for thermal conductivity, normalization/rescale of experimental data is more delicate and requires careful evaluation. In any case, satisfactory results are observed, with the correlation correction being consistent with the neighboring experimental data, which bends the correlation toward them. However, this case turns out to be more delicate, since the formula for thermal conductivity comes from a physical model, unlike the fuel melting temperature, which is treated with a purely empirical fit. Therefore, no firm conclusions can be drawn about this second case.

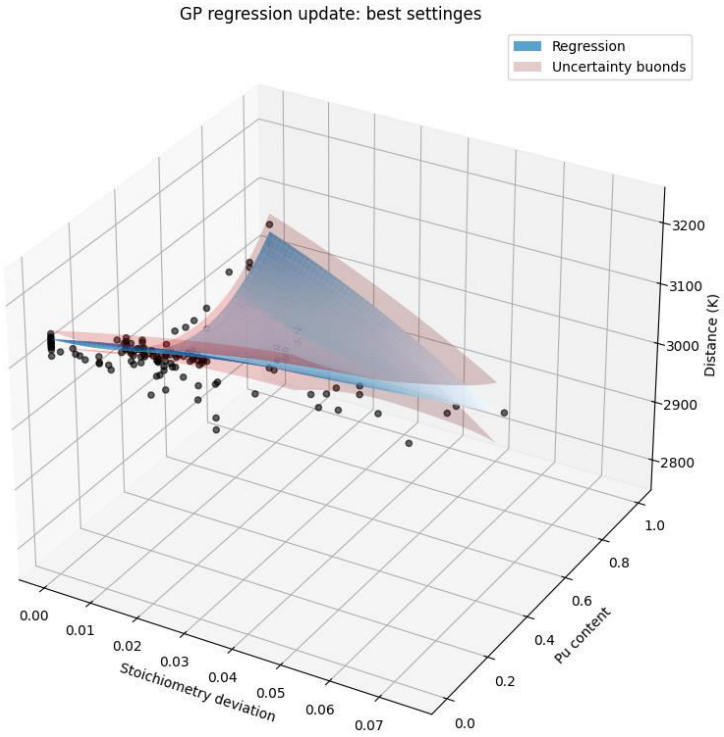

Figure 3.1: Fuel melting temperature (K) obtained with GP regression using the varying settings.

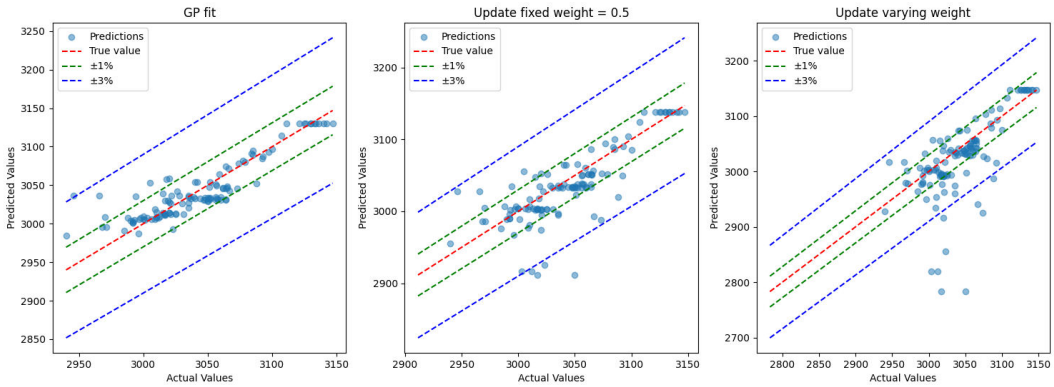

Figure 3.2: Fuel melting temperature (K) experimental values against predicted values for the pure GP fit, the correlation update with fixed weight equal to 0.5 and the correlation update with the weight varying with the stoichiometry deviation and the plutonium content.

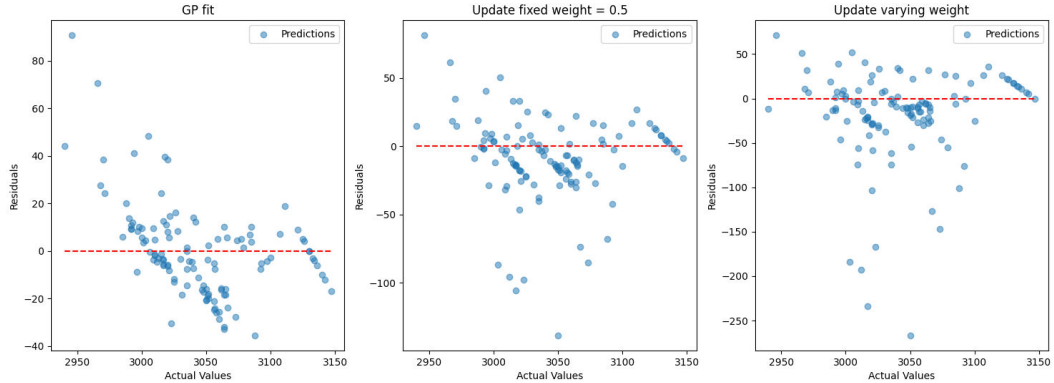

Figure 3.3: Fuel melting temperature (K) residuals values against predicted values for the pure GP fit, the correlation update with fixed weight equal to 0.5 and the correlation update with the weight varying with the stoichiometry deviation and the plutonium content.

4. Conclusions and Recommendations

A data assimilation method based on GP regression was implemented and an application for the MOX fuel melting temperature and its thermal conductivity is presented. The advantage of this type of tool is the ability to allow automatic management of data sets to provide codes with the necessary correlations (e.g., for material properties). It is possible, therefore, to think of an integrated tool that can comprehensively manage material properties in a way that is decoupled from the FPCs that one decides to use. This is a major advance in terms of nuclear data management since it avoids the need to perform continuous statistical analyses on them whenever new experimental values are available.

The only aspect that requires some special attention concerns the data preprocessing, which should be appropriately normalized and/or rescaled since regression routines provide better results for values that have similar orders of magnitude. In addition, it can be combined with clustering algorithms to handle large amounts of data, especially when we have many measurements made under the same conditions that provide different results (due to intrinsic uncertainty or errors in the measurement process). In this way, it is possible to clean up the data set by obtaining scattered data, but at the same time in a sufficient number to be able to perform a good quality regression.

It should also be emphasised that for quantities for which few data are available, such as those we consider in this work, it was not possible to perform a validation with a portion of the dataset other than that used for training. The generalisation of this approach towards validation will be discussed in a future work under preparation, as will the automatic choice of weights to perform the correlation update, the aim of this preliminary work being only to show the potential and possible uses of the method illustrated.

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