RS-HDMR-GPR Code Manual

Version 1.0.3

Coded by Owen Ren.

For the description of the method see the accompanying article:

Random Sampling High Dimensional Model Representation Gaussian Process Regression (RS-HDMR-GPR) for representing multidimensional functions with machine-learned lower-dimensional terms allowing insight with a general method

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Contents

This software is a Python implementation of the Random Sampling High Dimensional Representation Gaussian Process regression (RS-HDMR-GPR) method. It represent a multivariate function as a sum of lower-dimensional terms (component functions) constructed with Gaussian process regressions. All component functions are determined from a single set of arbitrarily distributed samples. The dimensionality and the numbers of terms can be selected for optimal fit quality. The code also permits imputation of missing data values based on the HDMR decomposition. The user is advised to read the accompanying article for the description of the method and the meaning of its key parameters (ref to preprint)

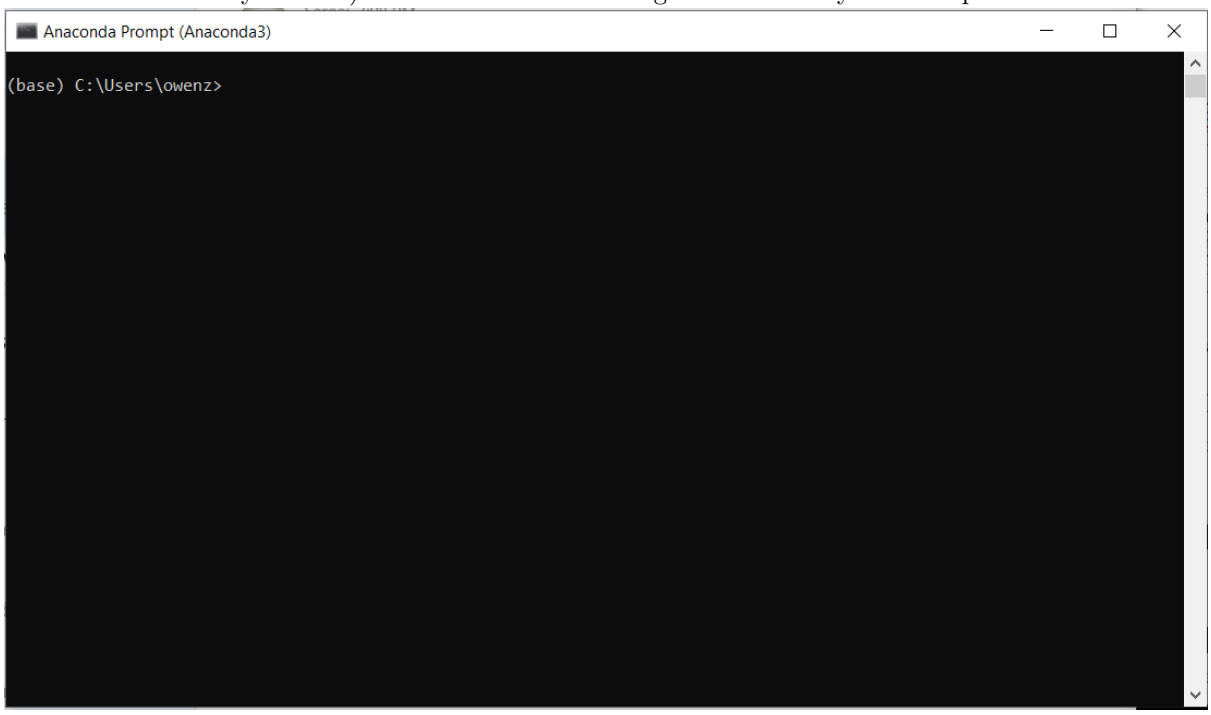
1 Installation Guide

The latest version of the code can be obtained from github and the user is advised to download the latest version. The code comes with a IPython jupyter notebook (examples.ipynb) that allows one to run and test the examples provided in the accompanying paper.

The **rshdmrgpr** package is installed as a Python package. Please install the 64-bit Python, pip which allows for package installations (you can install this after installing anaconda) and git (you can use default settings for all the install steps) on your machines. Please also install anaconda distribution to work with conda virtual environments (*anaconda software, jupyter notebook*). The code can also be run on google collab, or any environment that supports jupyter notebooks. In this section, we will only provide a windows installation guide because the authors have only worked on this package in Windows environment. However, there should not be anything that prevents a user from using the package on other operating systems (OS).

1.1 Anaconda Setup and Windows Installation

First for a detailed list of anaconda commands please see here. Once Anaconda is installed, please open up "Anaconda Prompt (Anaconda3)" (which can be found by typing it in the windows start menu and should also exist on your mac). It should look something like this once you have opened it:



You should first check that you have git installed first by typing

```
git --version
```

Something like

```
(base) C:\Users\owenz>git --version
git version 2.33.0.windows.2
```

should appear after you typed it. If not please install git here (you can use default settings for all the install steps). Also make sure you have pip installed. If not installed please install it by typing in

```
conda install -c anaconda pip
```

in anaconda prompt and you can similarly checking if it is installed by typing "pip –version" like this:

```
(base) C:\Users\owenz>pip --version
pip 19.2.3 from C:\Users\owenz\Anaconda3\lib\site-packages\pip (python 3.7)
```

Now once both git and pip are installed, create a conda environment with 'env_name' as any name of your choosing and 'python=3.6' the version of Python to install for this environment (or other versions if you prefer by changing 3.6. We recommend not going beyond 3.7 though because our code has not been developed in Python 3.8 or newer):

```
conda create -n env_name python=3.6
```

Activate the environment, which in this case is called 'env_name' (this can be named to the users choosing):

```
conda activate env_name
```

Install the rshdmrgpr package inside the conda environment:

```
pip install git+https://github.com/owen-ren0003/rshdmrgpr
```

Install jupyter lab:

```
conda install -c conda-forge jupyterlab
```

Finally, start jupyterlab to starting working interactively in a jupyter notebook:

```
jupyter lab
```

Note that all of the required packages should have been installed when you ran "pip install git+https://github.com/owen-ren0003/rshdmrgpr". If some of the required packages were missed, you can install them separately via "pip install" or "conda install". Please consult:

1. conda install package instructions.
2. pip install package instructions.

Note: To run the unittest, navigate to the rshdmrgpr folder and simply type (folder structure shown below as an example)

```
(research) C:\Users\owenz\Desktop\rshdmrgpr>pytest
```

If pytest is not installed, then you can install it using pip or conda command like all python packages. pytest MUST be installed to run the unittest via terminal. Otherwise a python IDE such as PyCharm needs to be installed and the test run from there.

2 Function Reference

The entire implementation is in a single Python script rs_hdmr_gpr.py which consists of six helper functions and two classes. The docstrings and descriptions for these helper functions and classes are given below. The implementation uses GaussianProcessRegressor class's implementation from the Python sklearn library. Each Regressor will act as component functions for our HDMR implementation. In order to train each GaussianProcessRegressor we need to provide kernels which are also defined in the sklearn library. In the next section, we describe in detail how to use this code.

2.1 Helper function `kernel_matrices`

Before working with the algorithm, we need to first load the data sets. The helper function load_data will load one of our three built-in datasets. They are respectively: the dataset sampled from the interatomic potential function of the water molecule (H_2O), the kinetic energy density (KED) dataset from physics, and a dataset with major financial indices, currencies and commodities of S&P 500.

`rshdmrgpr.load_data(dataset)`

This function is used to load one of our three built-in data sets as a pandas DataFrame.

Parameters

- **dataset:** `str` – Specifies which dataset to load. One of 'h2o', 'KED', 'financial'.

Returns

- `pandas DataFrame` – The desired dataset.

To conveniently create input parameters for training the standard k-dimensional HDMR models, the helper function kernel_matrices gives the user the option to return such parameters by specifying the dimension, order and the kernel to be used for training the RSHDMRGPR model. The returned lists of this function is used to initialize RSHDMRGPR class. For details on how this is used, please see next section.

`rshdmrgpr.kernel_matrices(order, dim, kernel_function=RBF, **kwargs)`

This function is used to create any list of kernels and matrices suitable as inputs for the training step of RSHDMRGPR class. The available list of kernels that can be used are given in kernels.

Parameters

- **order:** `int` – The order of HDMR to use.
- **dim:** `int` – The dimension of the feature space.
- **kernel_function: any kernel from sklearn.gaussian_process** – Any kernel used for GPR. Please see documentation on the available kernels. Default is RBF.
- ****kwargs: keyword arguments** – Arguments for the given GPR kernel.

Returns

- `list` **of 2D-**`numpy Array` – List of matrices (2D–numpy arrays), used to select the features to train the component functions. The list should have size equal to the number of component functions the user wants to use to train RSHDMRGPR model.
- `list` **of sklearn.gaussian_process kernels** – List of kernels to use for training the component functions. The list should have size equal to the number of component functions.

To supplement the RSHDMRGPR class, the helper function below allows for sequential fitting as in equations (5) and (6) in the accompanying paper. The inputs are a list of RSHDMRGPR instances to fit in the order of increasing order (dimensionality of terms). Each model is fit to the difference of the label minus the predictions of the previous models.

`rshdmrgpr.sequential_fitting(x_train, y_train, models, **params)`

This function fits a list of RSHDMRGPR models sequentially (please see equations (5) and (6) in the paper). Each model is fitted to the difference of the target minus the predictions of the previous models.

Parameters

- **x_train:** pandas DataFrame – The training set.
- **y_train: 1d - array** – The target vector.
- **models:** list **of RSHDMRGPR** – The list of RSHDMRGPR instances (of class RSHDMRGPR) to fit.
- ****params: dict** – variable number of key word arguments. Used to specify arguments for RSHDMRGPR.

Returns

- list **of 2D-**numpy Array – List of matrices, used to select the features to train the component functions. Has size $\binom{\text{dim}}{\text{order}}$, the number of ways to choose order from dim.
- list **of** RBF **kernels** – List of RBF kernels to use for training component function. Has size $\binom{\text{dim}}{\text{order}}$.

rshdmrgpr.**sequential_prediction**(*x_test, models*)

This function returns a list of predictions for each order of fit. The i-th (0-based index) element contains the sequential fits up to order i (i.e. the sum of the predictions from **model**$[j]$ for all $j = 0, 1, ..., i$). This is used in conjunction with sequential_fitting and essentially provides the prediction part to the fitting part.

Parameters

- **x_test:** pandas DataFrame – The data set to be predicted on.
- **models:** list **of RSHDMRGPR models** – Contains the list of RSHDMRGPR models to be fitted sequentially.

Returns

- list **of 1d-array** – The i-th element contains the sequential fits up to order i.

2.2 RSHDMRGPR class

This class is used to fit a single instance of an hdmr model. A single instance is the sum of component functions determined by the matrices argument (a list of numpy matrices) that determines the component functions via right multiplication with the feature matrix of a given dataset. To perform sequential fitting, we need a list of RSHDMRGPR models and fit each sequentially where successive models fit to the difference of the label and the sum of the previous model predictions. Please see the main article Section 1, equations 5 and 6 for details.

class rshdmrgpr.**RSHDMRGPR**(*matrices, kernels*)

Bases: object

This class initializes the RS-HDMR-GPR model.

Parameters

- **matrices:** list **of 2D** numpy Array – The matrices that define the HDMR component functions. Every matrix must have the same number of rows equaling the dimension of the feature space.
- **kernels:** list **of kernels** – The list of sklearn.guassian_process.kernels to use for each HDMR component function.

2.2.1 RSHDMRGPR class methods

RSHDMRGPR.**verbose_print**(*msg, end=None, on=True*)

Used to print messages during the train method execution. Used with the verbose argument.

Parameters

- **msg:** str – The desired message to print.
- **end:** None or str – Specifies the ending of a line.
- **on:** bool – Specifies whether to print or not. This is controlled by the verbose argument in the train method.

Returns None

RSHDMRGPR.**train**(*self, x_train, y_train, alphas=1e-7, n_restarts=1,cycles=50, scale_down=(0.2, 2), optimizer=None, opt_every=5,use_columns=None, initializer='even', report_loss=False, verbose=0*)

Trains the RS-HDMR-GPR model (trains all the GPR models – the component functions).

Parameters

- **x_train:** pandas DataFrame – The DataFrame containing the features.
- **y_train:** pandas Series – The Series containing the target values.
- **alphas:** int or (list of int) – The noise level to be set for the component functions, each of which is a GPR model. If int, the noise level for training each of these models is the set to this for all cycles. To set different noise levels for different component functions, a list of int must be specified. Note that if optimizer is used, these values will be optimized via a WhiteKernel.
- **scale_down:** tuple – Must be a tuple, say (s, e) of size two. Training predictions for each component function will be multiplied by $\min\left\{s+\frac{(1-s)ec}{T}, 1\right\}$ on cycle c, where T denotes the total number of cycles. This is used to prevent overfitting of a single component function.
- **cycles:** int – The number of self-consistent cycles to use for training.
- **optimizer:** str or (list of str) – Must be a GPR optimizer or list of such. If a list is provided, each component function will use the corresponding optimizer specified in the list. Please see the sklearn documentation for GaussianProcessRegressor optimizer.
- **opt_every:** int – Specifies that the optimizer will be applied every (opt_every) cycles. Default=1 (optimizer applied every cycle). The optimizer will always be applied to the first and last cycles. This argument provides no meaning if optimizer is None or a list of None.
- **use_columns:** list of bool or None – Specifies which column to use (True indicates use, false otherwise) for training. If None (the default) is provided, all columns are used.
- **n_restarts:** int – Positive integer indicating the number of restarts on the optimizer (this is a hyperparameter for GPR).
- **initializer:** list of float or 'even' – Initializes the starting targets for each component function. If 'even', every target is equal to y_train / len(use_columns).
- **report_loss:** bool – If True, saves the loss from the prediction on the training set over every cycle. Only RMSE (Root mean-squared error) loss is supported for now.
- **verbose:** int – Sets the various print details option during training. Takes on values 0, 1, or 2. Default is 0. A level of 2 shows the least detail and a level of 0 shows the most detail.

Returns self, pandas DataFrame – Returns only the trained instance of self if report_rmse=False, otherwise returns the trained instance of self and a DataFrame containing the rmse values.

RSHDMRGPR.**predict**(*test_data, return_std=False*)

Computes the output of the trained RSHDMRGPR model on a given data set.

Parameters

- **test_data:** pandas DataFrame – The DataFrame containing the features of the test set. Should have one less column than the data used for training.
- **return_std:** bool – If True, the sum of all the component functions standard-deviation of the predictive distribution at the query points is returned along with the mean.

Returns

- **y_pred: 1D-**numpy Array – Sum of the mean of predictive distribution at query points of all component functions.
- **y_std: 1D-**numpy Array – Sum of the standard deviation of predictive distribution at query points of all component functions. Only returned when return_std=True.

RSHDMRGPR.**get_models**()

Returns the trained RSHDMRGPR component functions. Model must be trained first.

Parameters None

Returns list **of** GaussianProcessRegressor – List of GaussianProcessRegressor from the sklearn.gaussian_process library, their trained instances.

2.3 FirstOrderHDMRImpute class

This class is uses 1D-HDMR trained RSHDMRGPR instances to impute data sets where each row has at most 1 missing value. It is important that the dataset satisfies this criterion, otherwise the code will not run or yield unexpected behaviour. The initialization of this class uses the trained models returned by get_models() method from the RSHDMRGPR class.

class rshdmrgpr.**FirstOrderHDMRImpute**(*models, division=1000*)

Bases: object

This class is used for imputation based on first order HDMR. The class is initialized by vectorizing the 1D-HDMR component functions and creating a dictionary of output values with division subdivisions. This is done because we need the inverse relation of each component function. This acts as a lookup table for inverse values where the endpoints of the subdivisions are inverse values. The larger the value of division, the more precise the inverse will be at approximating.

Parameters None

- **models:** list **of** GaussianProcessRegressor – list of trained GaussianProcessRegressor models which represents the hdmr component functions of first order. Must be of first order (each has 1 input and 1 output).
- **division:** int – The number of divisions in the lookup table

2.3.1 FirstOrderHDMRImpute class methods

The class below provides

FirstOrderHDMRImpute.**get_table**()

Returns the lookup table for the component functions.

Parameters None

Returns **panda** DataFrame – The lookup table for the HDMR component functions.

`FirstOrderHDMRImpute.`**`get_yi`**`(`*`df_na`*`)`

Modifies the `DataFrame` to contain the output columns of the first-order hdmr component functions. The output columns are concatenated after the last column of `df_na`. The DataFrame in question should have missing values and for each row there should be at most one missing value.

Parameters None

- **`df_na:`** `pandas DataFrame` – The `DataFrame` to impute. Must contain the output column and that column must be the last column.

Returns `list` – `list` of column indices for each row having a missing value (of `df_na`).

`FirstOrderHDMRImpute.`**`impute`**`(`*`df_na, get_candidates=False, threshold=0.001`*`)`

This function imputes the missing values given the input. Every single input row is expected to have at most one missing value.

Parameters None

- **`df_na:`** `pandas DataFrame` – The `DataFrame` to impute. It is expected to contain the columns corresponding to 1D hdmr outputs (i.e. as an output of the `get_yi` function).
- **`get_candidates:`** `bool` – If True, returns all the candidates for imputation.
- **`threshold:`** `float` – The threshold distance to set for selecting candidates from look-up table. Correspond to δ in the paper (Section 2.2).

Returns

1) `pandas DataFrame` – The imputed `DataFrame df_na` if `get_candidates=False`.
2) `pandas DataFrame`, `pandas Index`, `pandas Series`, `list` **`of`** `float` – The imputed `DataFrame df_na`, the index of rows with null entries, the column names (indexed by the index of null entries) containing the null entry, and a list of candidates for imputing that missing value if `get_candidates=True`.

3 Usage

The function docstrings were given in the previous section. The present section serves as a tutorial on how to invoke these functions and classes.

3.1 Training RSHDMRGPR

As a first basic example, we fit a three-dimensional dataset which is obtained by sampling the interatomic potential of H_2O which is one of the build-in datasets for this package. The first thing we need to do is import the required packages to begin our analysis.

```
import numpy as np
import pandas as pd

from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import MinMaxScaler
from sklearn.model_selection import train_test_split
from sklearn.gaussian_process.kernels import *

from rshdmrgpr.rs_hdmr_gpr import *
```

Next, we extract the dataset via the helper function `load_data`

```
data = load_data('h2o')
print(data.shape)
```

```
(10001, 4)
```

```
data.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 10001 entries, 0 to 10000
Data columns (total 4 columns):
 #   Column  Non-Null Count  Dtype
---  ------  --------------  -----
 0   a1      10001 non-null  float64
 1   a2      10001 non-null  float64
 2   a3      10001 non-null  float64
 3   out     10001 non-null  float64
dtypes: float64(4)
memory usage: 312.7 KB
```

The dataset consists of 4 columns where the first three columns are features and the last columns is the target. To run RS-HDMR-GPR, we need to re-scale the dataset linearly so that the columns are between $[0, 1]$. (Alternatively any re-scale method works). We do this using MinMaxScaler from the sklearn package.

```
scale = data['out'].max() - data['out'].min()  # Keep the original scales for the target column
scaler = MinMaxScaler(feature_range=(0, 1))  # Initializes MinMaxScaler instance
scaler.fit(data)  # Fits the instance to the current dataset
# Transforms the data set to be between [0, 1]
data_scaled = pd.DataFrame(scaler.transform(data), columns=['a1', 'a2', 'a3', 'out'])  # The ↘
    transformed data set.
```

After transforming the dataset, we are now ready to split for training and prediction. Our training set will consists of 1000 rows and our test set will be the entire PES dataset. We split the data using `train_test_split`.

```
x_train, x_test, y_train, y_test = train_test_split(data_scaled.drop(columns=['out']), data_scaled['↘
    out'], train_size=1000, test_size=None, random_state=42)
```

In order to initialize RS-HDMR-GPR class we need the list of matrices and kernels to be used to define and train the component functions. We start with training the 1d-hdmr-gpr model. First we call the helper function `kernel_matrices` to quickly give us the matrices and kernels. Any kernel from `sklearn.guassian_process.kernels` will work, provided that the hyperparameters arguments are entered in the function as keyword arguments. For this case, we will use RBF kernels each with length scales of 0.6. Ideally, `length_scales` between 0 or 1 is desired as the starting input. However, the starting values for length_scale may not really be very relevant if the user decides to utilize the optimizer during training. Doing so will automatically search for the best `length_scales` for every component function over the cycles of fit.

```
matrices, kernels = kernel_matrices(1, 3, kernel_function=RBF, length_scale=0.6)
print(matrices)
print(kernels)
```

```
[array([[1.],
        [0.],
        [0.]]),
 array([[0.],
        [1.],
        [0.]]),
 array([[0.],
```

```
        [0.],
        [1.]])]
[RBF(length_scale=0.6), RBF(length_scale=0.6), RBF(length_scale=0.6)]
```

We can see that there are three matrices in the list each corresponding to a standard basis vector of $\mathbb{R}^3$. Each of these matrix is left multiplied with the data set to give only the column corresponding to the 1. For details, please see accompanying document, section 2.1, for more details. With the matrices and kernels we can initialize the class and train the model on the training set:

```
hdmr = RSHDMRGPR(matrices, kernels)
hdmr.train(x_train, y_train)
```

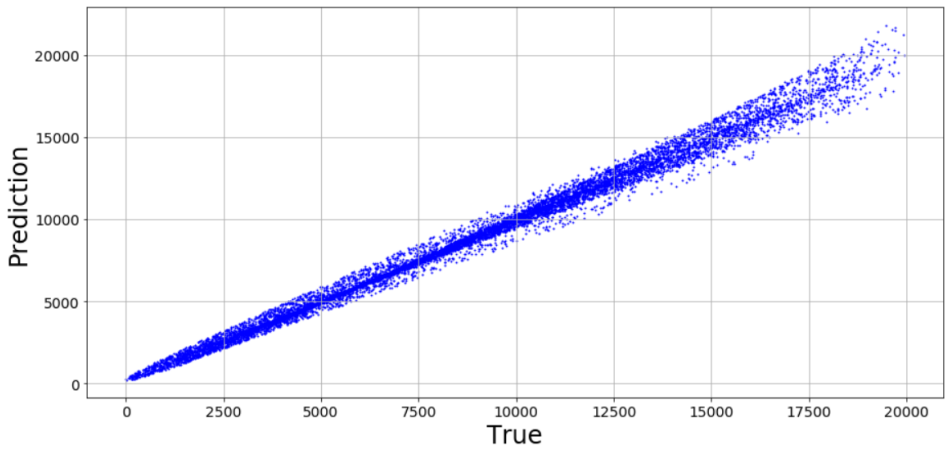
After training, we predict on the entire data set

```
y_pred = hdmr.predict(data_scaled.iloc[:, :3])
```

The correlation plot between the true values vs the predicted values is shown below:

```
correlation_plot(data_scaled["out"] * scale, y_pred1 * scale, xlabel='True', ylabel='Prediction', ↘
    figsize=(15,7))
```

```
Root mean squared error: 452.88959847675716
```



In this example, we used the default parameters for training. The user has control of 8 hyperparameters: scale_down, optimizer, n_restarts, alphas, cycles, use_columns, opt_every, and initializer that accounts for overfitting/regularization and other tasks. The `alphas` argument is important as it controls the nosie level for each GPR model during the fit. It can either be a single number which is the shared noise level for all the component GPR models or a list of values, one corresponding to the noise level for each model. The other hyperparameters are described in the section on Function References. We won't go into detail here as they are explained in the docstrings as well as the accompanying document. However, we have attached a notebook that explains each of these parameters in detail as a part of the supporting information. For further details, please see Section 5 of this manual.

3.2 1D - HDMR imputation

We demonstrate how the imputation class works on a synthetic example. The imports are the same as the previous subsection, so we omit the import code. We create a synthetic data set having 3 feature columns and a target column that is the sum of these three features:

```
def f0(*args):
    sumed = 0
    for a in [*args]:
        sumed += a

    return sumed

column_names = []
n = 3
for i in range(n):
    column_names.append(f'a{i}')
np.random.seed(42)  # Fixes the random seed so the results are always the same.
data = pd.DataFrame(np.random.rand(10000, 3), columns=column_names)
inputs = [data.iloc[:, i] for i in range(n)]
data['out'] = f0(*inputs)

# Scales the data to be between [0, 1]
scale = data['out'].max() - data['out'].min()
trans = data['out'].min()
data['out'] = (data['out'] - trans) / scale
```

```
x_train, x_test, y_train, y_test = train_test_split(data, data['out'], train_size=400, test_size=None,↘
    random_state=42)
```

We train the model on 100 points and set 300 of them aside for imputation. For these 300 points the first 100 rows have their first column set to missing, the second 100 rows have the second column set to missing, and finally the last 100 rows have the third column set to missing.

```
# Setting up DataFrame to be imputed.
df_na = x_train[100:].copy()
df_na.iloc[:100, 0] = np.nan
df_na.iloc[100: 200, 1] = np.nan
df_na.iloc[200: , 2] = np.nan
```

Now we initialize first order imputation class. This class must be initialized

```
foimp = FirstOrderHDMRImpute(gpr.get_models())
```

In order to impute for the missing values, we need to compute the outputs of the component functions and append it to the DataFrame.

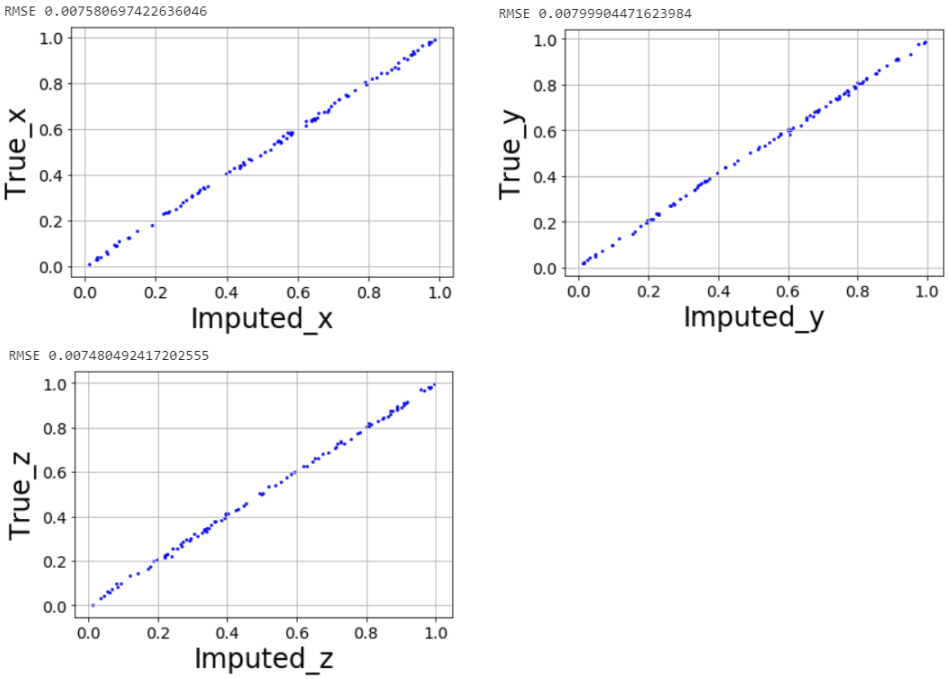
```
# Appends the output columns for the component functions
foimp.get_yi(df_na)
```

With these output values from the component functions, we now impute the missing values.

```
# Imputes the missing values
foimp.impute(df_na)
```

Finally, with the imputed values, we show how close they are compared to the actual values.

```
labels = ['x', 'y', 'z']
for i in range(3):
    correlation_plot(df_na.iloc[100*i: 100*(i + 1), i], x_train.iloc[100*(i+1): 100*(i+2), i], xlabel=↘
        f'Imputed_{labels[i]}', ylabel=f'True_{labels[i]}')
```



4 UI

We have created a graphics user interface using Python Tkinter package to help assist user with using the code. This sections helps walkthrough the user on it's use. To run the UI, go to terminal and run the file ui.py inside rshdmrgpr package via Python. For example,

```
C:\Users\new_user\rshdmrgpr>python ui.py
```

Note, it is important that all of the respective files in the package are there when running this script. The UI is broken down into four parts, as shown in the Figure 1 below: The four steps represent the

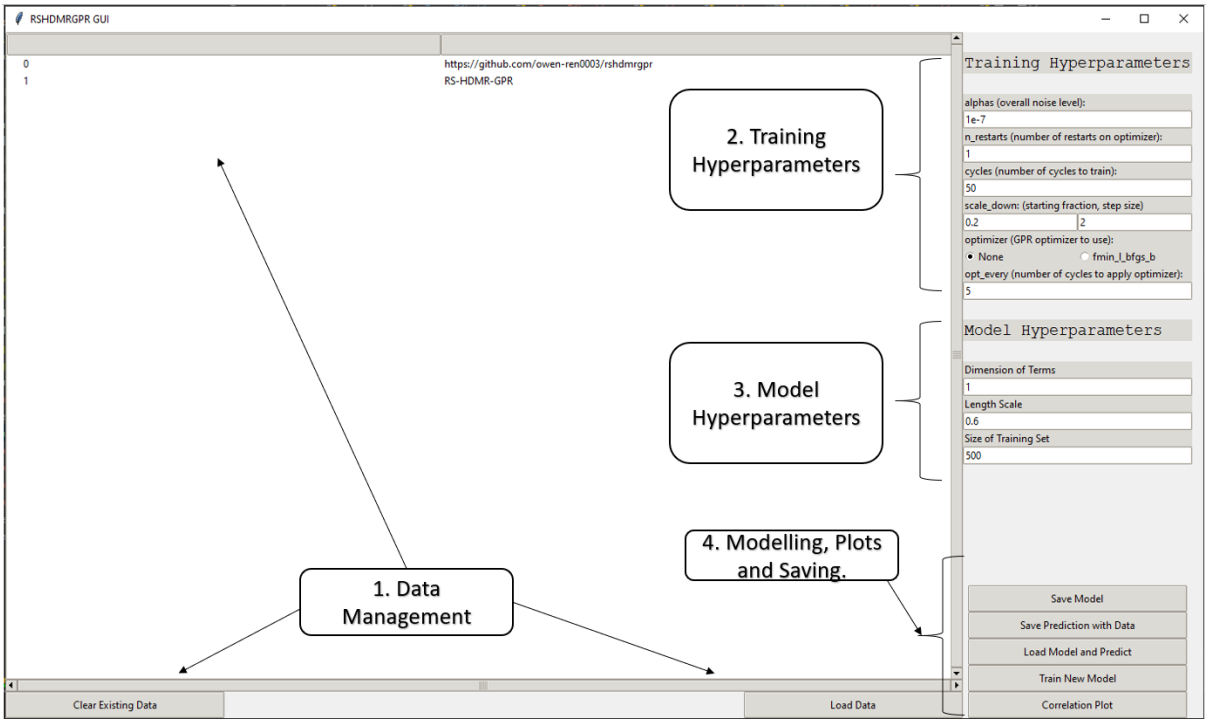


Figure 1: GUI main window overview.

suggested order of execution the user should follow in order to use the GUI efficiently. These steps are listed below:

1. Data Management - Loads a new data set. This new data set should be vertically structured and should have one of the extensions (.txt, .csv, .xlsx, or .dat).

2. Specify Training Hyperparameters - These are a subset of hyperparameters of the train function in class RSHDMRGPR that must be specified (although default values are provided) to start training.

3. Specify Model Hyperparameters - These are model hyperparameters that must be specified prior to training. These include: The order of hdmr (dimensionality of its component functions), the length scale of the kernel used, and the size of the training set.

4. Modelling, plotting and saving - These are buttons to initiate training, prediction, saving/loading models, and plotting the correlation plot between predicted and actual values.

We go over these steps in detail in the next part.

4.1 Data Management

This part is simple, there are two buttons that performs loading of new data and clearing of data that has been loaded. It is important to note that data must be vertically structured, that is, the rows represent individual entries of the data, and the columns specify the data features.

The files that can be loaded included .txt, .csv, .xlsx or .dat files. They should be comma separated comma separated.

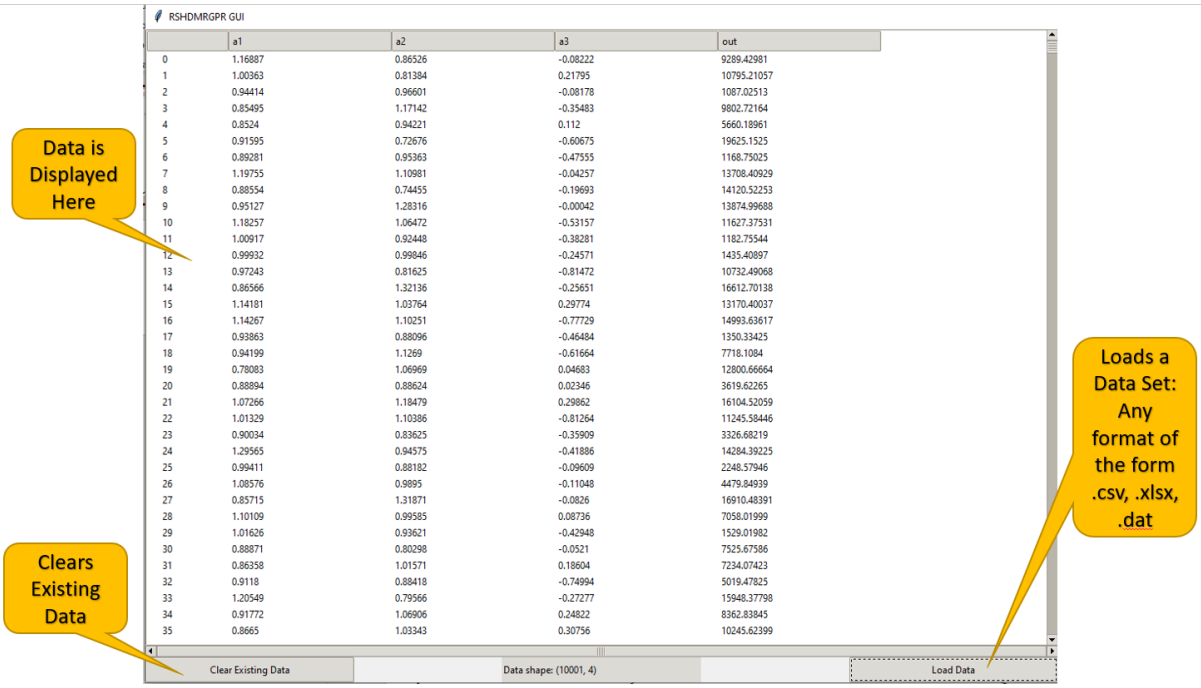


Figure 2: GUI main window overview.

4.2 Specifying Training and Model Hyperparameters

After data is loaded, there are two sets of configurable parameters that must be specified before training can start. The first set of parameters is used to train the RS-HDMR-GPR model. These are a portion of the parameters specified in the train function of RSHDMRGPR class. Their description are given in Section 2. The second set of parameters are used for model. There are three parameters to configure. The default parameters if the user does not want to specify. These are listed and described below:

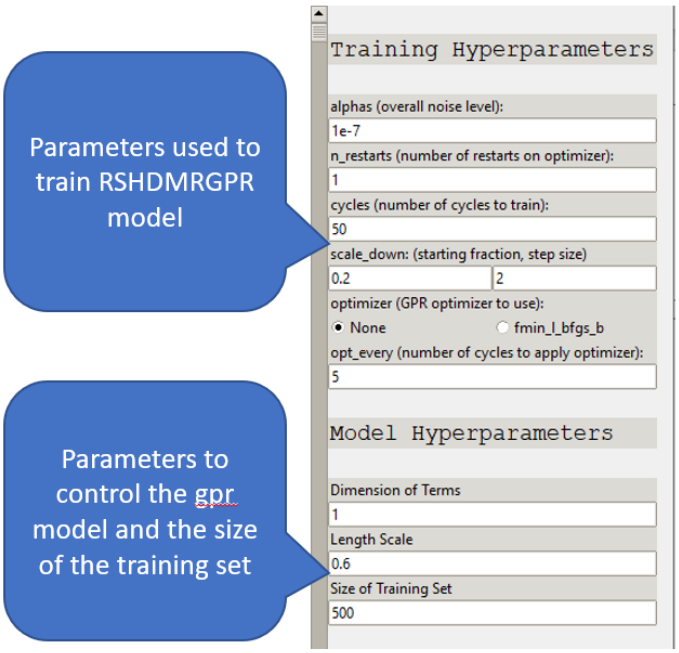


Figure 3: GUI main window overview.

1. Dimension of Terms – The order of HDMR to use.
2. Length Scale – The length scale used for GaussianProcessKernel kernel
3. Size of Training Set – The number of data entries used for training. The complementary set is the test set.

4.3 Modelling, Plotting and Saving

Once the data has loaded and the parameters set, next we are given several options as shown in Figure 4. We describe each option in detail

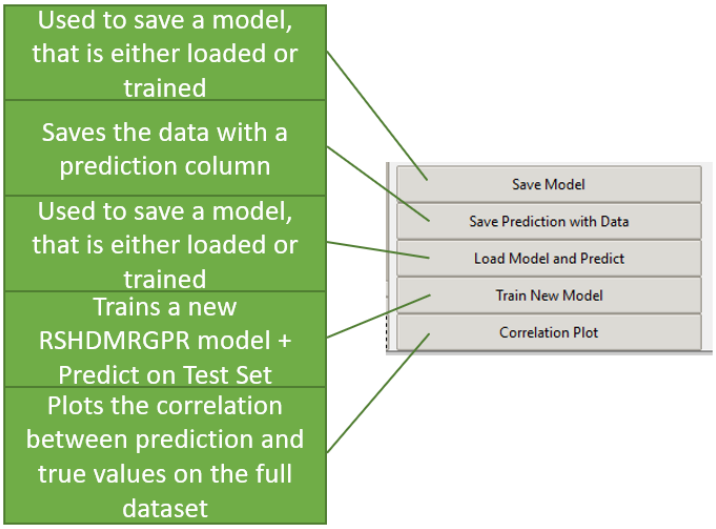


Figure 4: GUI main window overview.

1. Save model – Saves the trained or loaded model as a pickle (.pkl) file.
2. Save prediction with data – Adds the prediction column to the data and saves the data as a .csv file
3. Load model and predict – Loads a model that is saved as a pickle file and predicts on the loaded data.
4. Train new model – Trains a new GPR model and predicts (on the test set) using specified parameters on the dataset.
5. Correlation plot – Plots the correlation graph between the predicted and actual values.

5 Algorithms

This section explains the implementation of the following three algorithms in pseudo-code format: The RS-HDMR-GPR algorithm, the aglorithm for sequentially fitting the RS-HDMR-GPR models, and the imputation using 1D-HDMR. Notations:

1. m – number of entries for the data.
2. n – number of features the data contains.
3. $\alpha(c)$ – A scale down function as a function of the cycle number c.
4. $P_\ell(i)$ – A permutation of $\{1, 2, \ldots, \ell\}$ applied to element i.
5. X denotes a $m \times n$ matrix containing data corresponding to the features.
6. y denotes a $m \times 1$ vector containing the target data.

Algorithm 1: RS-HDMR-GPR

Input:

1. ℓ matrices $A_1, A_2, \ldots, A_\ell$, each of size $n \times k$.
2. GPR kernels K_i for $i = 1, 2 \ldots, \ell$. (Usually successive orders of HDMR. The kernels supported for now are RBF and Matern. For this, the noise level and length scales needs to be provided as user inputs. Both anisotropic and isotropic kernels work).
3. The feature matrix X and label vector y.
4. A scale–down function $\alpha(c)$.

Output: Trained RS-HDMR-GPR model

Initialize vectors $\vec{y}_i = \frac{1}{\ell}\vec{y}$ and GPR models $\mathbf{model}_i = \varnothing$ for all $i = 1, 2, \ldots, \ell$.
Set P_ℓ to be the identity permutation. **for** $1 \leq c \leq$ # cycles **do**
  for $1 \leq i \leq \ell$ **do**
    1. Train $\mathbf{model}_{P(i)}$ using kernel $K_{P(i)}$ with input $XA_{P(i)}$ and output $\vec{y} - \sum_{j \neq P(i)} \vec{y}_j$.
    2. Update $\vec{y}_{P(i)} :=$ ($\mathbf{model}_{P(i)}$'s prediction on $XA_{P(i)}$) $\times\, \alpha(c)$
    3. Update $K_{P(i)}$ parameters to trained $\mathbf{model}_{P(i)}$'s new length scale if optimizer is applied.
  Choose a random permutation P_ℓ if permutation option is choosen.

For Algorithm 1, we did not include the various parameters from the implementation. These are explained in the accompanying notebooks.

Algorithm 2: Sequential Fitting

Input:

1. A list of untrained RS-HDMR-GPR models: $\mathbf{model}_i$ for $i = 1, 2, \ldots, k$.
2. The feature matrix X and label vector y.

Output: Trained instances of $\mathbf{model}_i$ for $i = 1, 2, \ldots, k$.

for $1 \leq i \leq k$ **do**
  Train $\mathbf{model}_i$ with respect to X and $\vec{y}$
  update $\vec{y}$ to $\vec{y} - \vec{z}$ where $\vec{z}$ is the prediction of $\mathbf{model}_i$ on X.

Algorithm 2 takes a collection of RSHDMRGPR instances and fits them in the order they are given. It is done via the `sequential_fitting` function from the code. The function `sequential_prediction` is used to predict for after sequential fitting is performed. Please see API and the notebook in SI for further details.

Algorithm 3: First order RS-HDMR-GPR imputation

Input:

1. 1D-HDMR component functions $f_1, f_2, \ldots, f_n$
2. A $m \times n$ feature matrix X whose columns entries are scaled to be between $[0, 1]$. For each row of X, there is at most one entry that is missing.
3. An integer $d > 0$.

Output: A $m \times n$ feature matrix X' that has it's missing values imputed

Compute the lookup table for the f_i's with d subdivisions of $[0, 1]$.
for *each row r of X with index i having a missing value* **do**
    Compute $y_i = \vec{y}_i - \sum_{j \neq i} y_j$
    Determine a list of input values in the lookup table closest to or within $\frac{2}{d}$ of y_i.
    The first element from this list is used for imputing the missing entry.

For Algorithm 3, it is important that input data matrix contains at most 1 missing value per row. The method implemented only works only for this case.

6 rshdmrgpr Examples

The supplementary IPython jupyter notebooks (examples.ipynb and physics_example.ipynb) demonstrates in detail how to use this package on the built-in datasets. We have tried to make the examples sufficiently comprehensive to demonstrate different ways of code usage for its various capabilities. That is we explain through these examples the various hyperparameters and code usages of RS-HDMR-GPR implementation. All of the examples presented in the accompanying document are worked out in these notebooks.