Gaussian Process Regression Machine

Project Report

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I, the undersigned, hereby declare that the work contained in this report is my own original work unless indicated otherwise.

Signature Date

Summary

It is often the case that there are systems which has multiple variables. In certain cases the value of one of the variables are unknown when the values of all the other variables are known. In this study we aimed to investigate and implement the use of regression for predicting the unknown value using both linear and kernel (non-linear) methods. We started with direct linear regression. From there we progressed to Bayesian linear regression to determine predictive distributions. After that we investigated the relation between linear regression and kernel-based methods. Finally, we used the kernel-based method on its own and also applied them to Gaussian processes. We tested the predictive methods with both simulated as well as real-life data.

Dit is dikwels die geval dat daar stelsels is wat verskeie veranderlikes het. In sekere gevalle is die waarde van een van die veranderlikes is onbekend wanneer die waardes van al die ander veranderlikes bekend is. In hierdie studie was daar gepoog om te ondersoek en te implementeer die gebruik van regressie vir die voorspelling van die onbekende waarde deur die gebruik van beide lineêre en kern (nie-lineêre) metodes. Ons het begin met 'n direkte lineêre regressive. Van daar het ons gevorder na Bayesiese lineêre regressie om voorspellende verspreidings te bepaal. Daarna het ons die verhouding tussen lineêre regressive en kern gebaseerde metodes ondersoek. Laastens het ons die kern gebaseerde metode op sy eie gebruik en ook toegepas op Gaussiese prosesse. Ons het die voorspellende metodes getoets op beide gesimuleerde en werklike data.

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List of Symbols

C	covariance matrix
D	dimensionality
M	basis function ticks for each dimension (i.e. M^D basis functions)
k	kernel function
k	column matrix of kernel function
K	Gram Matrix
t	the output value of a corresponding x vector
t	column vector of the output values of the training data
x	a vector of n values defining a location on the n-dimensional input space
x	a column vector of different x points
α	parameter
β	variance parameter
δ	Dirac delta function
θ	parameter
σ	variance
ϕ	basis function
Φ	design matrix
ω	function weight

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1. Introduction

The goal of this project was to investigate and implement the use of regression for predicting future values of a signal using both linear and kernel (non-linear) methods. We will progress from direct linear regression, through Bayesian linear regression and finally Gaussian Processes. We will test with both simulated as well as real-life signals.

The problem statement is as follows. Often it is encountered that there is a scenario in which there is an output parameter and one or more continuous input parameters. An estimation needs to be made of the output value for a point on the input space (the test input point) for which it is not possible to determine the output empirically. Thus, it is necessary to employ mathematical techniques to determine a probability distribution of the output at that input point. In order to do so, one needs to first have a data set of known output values and their corresponding points on the input space. These points are will be used as the training data. These training data will be fed to the mathematical model so that it can "learn" how each input parameter affects the output. The mathematical model can then be employed to make a prediction.

In this project, two such techniques were implemented and tested. The first of these is the predictive distribution for linear regression. It involves the definition of basis functions over the relevant part of the input space. The technique can then be used to determine to what degree each of the basis functions determine the output parameter. The weights that were assigned to the basis functions can then be used to determine a prediction of a test point.

The second technique that was used is called Gaussian processes for kernel regression. It involves the use of a carefully chosen kernel function that relates one training point to another. The kernel function has to be evaluated for each possible pairing of training points. This can then be used in an algorithm to make predictions for the test points.

Both of these regression methods were implemented in python. It was done using the Jupyter Notebook software in the WinPython package. It was set up in various Jupyter notebook files. All figures in this report were generated by python code we wrote ourselves. Both of the regression methods were tested on simple synthetic one-dimensional data to evaluate the functionality of the written code and its performance on simple data set. All the performance evaluations were done with a computer with a 2.2 GHz processor with four threads. It was then tested on more complex data and finally on real data sets. The results were evaluated, conclusions were drawn, and recommendations were made.

2. Literature Study

The study leader recommended some pieces of literature. We examined them and identified sections relevant to this project. *Pattern Recognition and Machine Learning* [Bishop, 2006] contains most of the mathematics that will be necessary for this project. The mathematical knowledge necessary to understand the content of this book is sufficiently satisfied by the knowledge gained in an undergraduate engineering course.

Chapters 3 and 6 contain the most important theoretical material that was used to write the software needed. Chapters 1 and 2 provide mathematical development that is necessary to understand the content of chapters 3 and 6. In particular, chapter 2.3 contains a very detailed explanation of the Gaussian distribution.

Chapter 3 explains linear models for regression. It starts with an explanation of explains how to set up models of basis functions. Section 3.3 explains Bayesian linear regression, which is one of the goals of this project. The subsection starts with parameter distribution for linear regression and illustrates how it works.

After that the predictive distribution for linear regression is also explained and illustrated. Derivations of the underlying mathematical formulae are provided. An explanation is given of how training data can be fitted to the basis functions in order to make predictions with Gaussian distributions. After that Bishop explains how kernel equivalents can be determined for basis functions. There is also a section on how to use evidence approximation, which appears to be a means of optimising the predictive distribution.

Chapter 6 explains how kernels can be constructed and how it can be used in regression. The chapter starts by further elaborating on how basis functions have a kernel equivalent in what is called a dual representation. An explanation is given on how it is possible to construct kernels without basis functions what rules needs to adhered to in this construction.

Section 6.3 explains radial basis functions, which works similar to the basis functions mentioned earlier. An exception that it is now based on the training points instead of being arbitrarily defined.

Section 6.4 explains how Gaussian processes can be applied to kernel regression. The equations for determining the means and variances of test points are derived. A means of optimizing the kernel function used by this prediction method is presented.

Chapter 45 in Mackay's *Information Theory, Inference, and Learning Algorithms* is also applicable. It includes the mathematics of Gaussian processes for kernel regression, except with different notation.

3. Linear Regression

3.1.Introduction

In this chapter, we document our analysis of linear regression and the experiments we did with it. Linear regression involves defining arbitrary basis functions over the input space. In this chapter, we explain how we selected suitable basis functions for the kind of data we analysed. We examined both the parameter distribution and the predictive distribution of linear regression.

The primary focus will be the predictive distribution. We show how the underlying mathematics of this distribution is derived. We tested it on both synthetic data sets and real world data sets and examined the results. All the used mathematics in this section is described in *Pattern Recognition and Machine Learning* [Bishop, 2006]. All the figures in this section were generated by python code we wrote ourselves. Some of them were generated in a way that attempts to mimic figures in the aforementioned source.

3.2.Parameter Distribution

First we demonstrate how an output that is a sum of weighted functions can be solved. The weights are iteratively improved until they converge. This is called the parameter distribution method for linear regression.

A two-dimensional multivariate Gaussian distribution was used as the prior distribution for this method. A two-dimensional input array over weight space was defined in python. The points in the input array correspond to a row-by-row grid of the pixels in figure 1. The probability of each output point is defined as one-dimensional vector in which the value of each entry is the relative probability of the corresponding input point. The values of each point on the probability array are shown as the colour on the corresponding input value's pixel. Warmer colours correspond to areas of larger values on the output array.

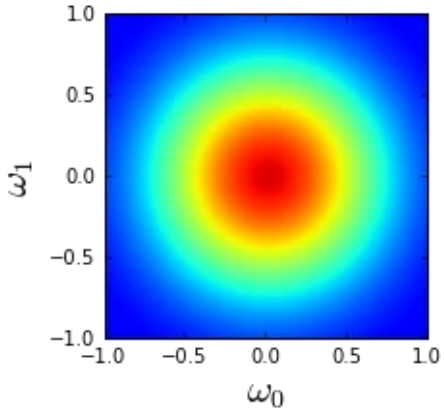

Figure 1: The prior distribution used for our demonstration of the parameter distribution method.

A python function, called heatmap_random, was written to select randomly select a point on this space with a probability equal to its percentage of the total probability of all the points. For this demonstration, the output is be defined by equation (1).

$$y = \omega_0 + \omega_1 x \tag{1}$$

Below is an evaluation of equation (1) for six random samples.

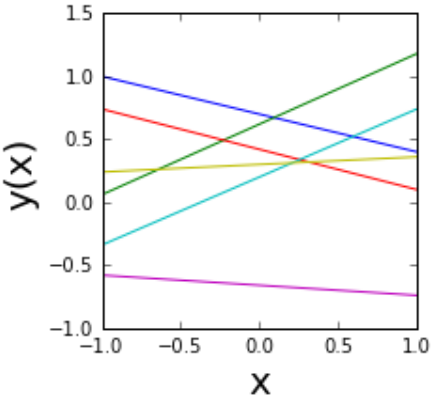

Figure 2: Equation (1) evaluated and plotted for six points on the weight space, selected with the heatmap_random function.

A point x on the x-axis is uniformly randomly selected on the interval [-1, 1]. Then for that point equation (2) is evaluated.

$$y = -0.3 + 0.5x + Normal(0, 0.2) \tag{2}$$

The equation shows that the actual values of ω_0 and ω_1 are -0.3 and 0.5 respectively. In this scenario, these two values are unknown and the parameter distribution method is used to recover it.

Using the particular random values of x and t that were selected, we determine and plot the probability of equation (1) over ω space, as shown on the left in figure 3. We then define a probability array for this image in the same way that the probability array for figure 1 was defined. This new probability array is then multiplied with the prior probability array to yield the distribution shown in the centre of figure 3. We then again generate samples from the weight space using the heatmap_random function, shown on the right.

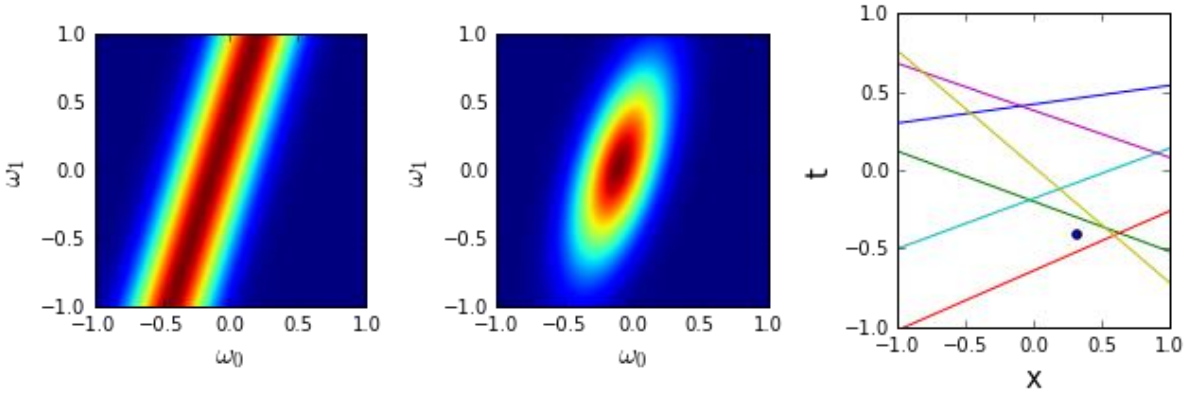

Figure 3: The steps in an iteration of the parameter distribution method. On the left is the pobability over weight space that equation (2) is true if x and t are evaluated to the point shown on the right. The plot in the centre, the new probability distribution over weight space, is the product of the plot on the left and the previous probability distribution over weight space.

This process can be repeated as many times as desired, each time using the new probability array as the prior. Below are the results after 20 iterations.

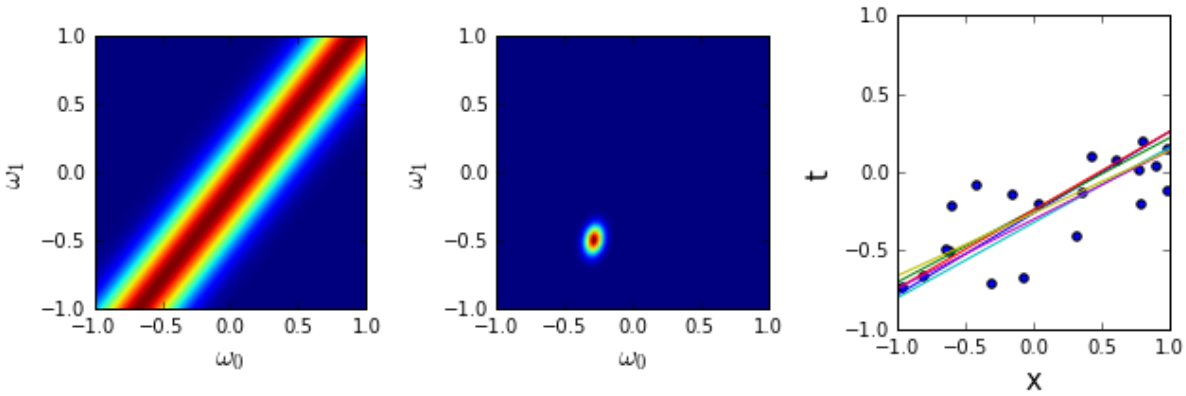

Figure 4: The same information shown in figure 3, except that this is the 20th iteration. The points that were randomly selected in each iteration is shown on the right.

This particular illustration is for the case of a one-dimensional input space and a single basis function. This method is not limited to these constraints, but a higher dimensional input space will require an exponentially larger number of computer calculations.

3.3.Predictive Distribution

3.3.1. One-Dimensional synthetic data

The predictive distribution method for the case of a one-dimensional synthetic input was implemented as described in here.

Here we aim to replicate the example in chapter 3.3 in Bishop's book. The code that is necessary to do so was implemented, but in such a way that it can easily be changed to accommodate multi-dimensional input, as will be necessary in a further demonstration.

The input x of the training data in this demonstration is 25 evenly spaced points on the interval [0, 1]. We assemble the vectors of these input points into a column vector denoted **x**, which is called the training input. The output is a sinusoid with Gaussian noise having a variance of 0.2, as shown in figure 5. The values of the output for each of these input points can be assembled into a corresponding column vector, denoted by **t**.

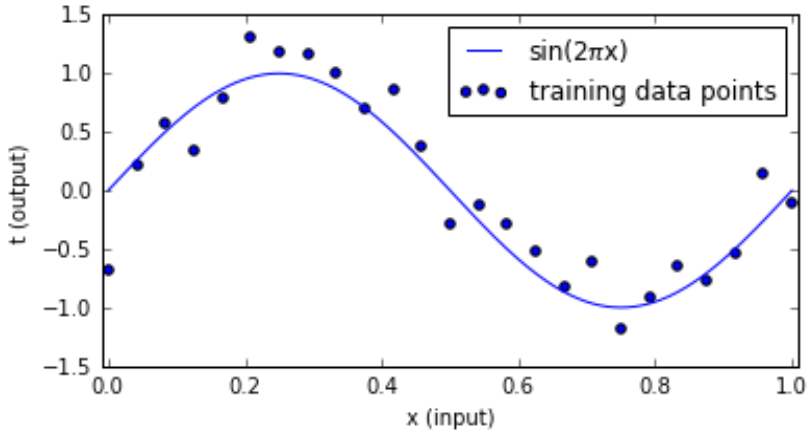

Figure 5: The training points used for the demonstrations in this chapter and the function they are derived from.

The basis functions that will be used for this demonstration consists of nine Gaussian distributions with means evenly spaced over the interval [0, 2] and each have variance of 0.2. We chose these basis functions because it is well spread over the area of interest, but not overly so. They are shown in figure 6

$$\phi_j(x) = exp\left\{-\frac{(x-\mu_j)^2)}{2s^2}\right\} \tag{3}$$

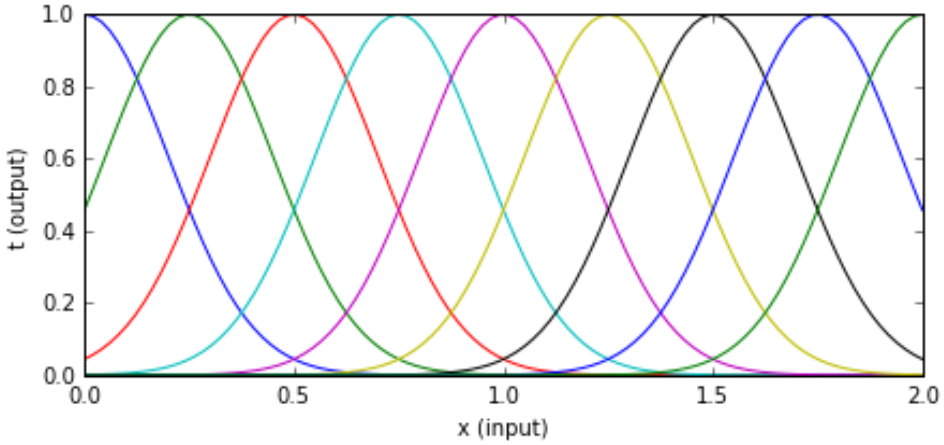

Figure 6: The basis functions for the predictive distribution method demonstration in this chapter.

For this demonstration the hyperparameters α and β are arbitrarily chosen to be one and five. α and β were chosen based on randomly trying different values until values that works well were found. Specifically, the values were α = 1 and β = 5.

Each of the basis functions can be defined for each of the training data points. These definitions can be assembled into a matrix called the design matrix, denoted by Φ. It is shown in equation (4). We also define S_N, which is necessary for further calculations.

$$\mathbf{\Phi} = \begin{pmatrix} \phi_0(\mathbf{x}_1) & \phi_1(\mathbf{x}_1) & \cdots & \phi_{M-1}(\mathbf{x}_1) \\ \phi_0(\mathbf{x}_2) & \phi_1(\mathbf{x}_2) & \cdots & \phi_{M-1}(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(\mathbf{x}_N) & \phi_1(\mathbf{x}_N) & \cdots & \phi_{M-1}(\mathbf{x}_N) \end{pmatrix} \tag{4}$$

$$\mathbf{S}_N^{-1} = \alpha\mathbf{I} + \beta\Phi^{\mathsf{T}}\Phi \tag{5}$$

After that a test data set is required. Unlike the training data set, only the input vectors of the test set have to be provided. There is no need to assemble all he test input vectors into a vector, because the prediction for each test point is made independently from the others. For this demonstration, we define the test vectors as a set of many evenly spaced points over the interval [0, 2].

We now have everything we need to evaluate the means and variances of the prediction. Equations (6) and (7) are the formulae for evaluating it. The probability distribution for each test point, defined in equation (8), of the prediction is a Gaussian distribution defined over the output axis.

$$\mathbf{m}_N = \beta\mathbf{S}_N\Phi^{\mathsf{T}}\mathbf{t} \tag{6}$$

$$\sigma_N^2(\mathrm{x}) = \frac{1}{\beta} + \phi(\mathrm{x})^T\mathbf{S}_N\phi(\mathrm{x}) \tag{7}$$

$$p(t|\mathrm{x}, \mathbf{t}, \alpha, \beta) = \mathcal{N}(t|\mathbf{m}_N^T\phi(\mathrm{x}), \sigma_N^2(\mathrm{x})) \tag{8}$$

The result of the prediction is shown in figure 7. This method evidently works well with for the given hyperparameters. We attempted to implement a means of calculating the most optimal hyperparameters, but were unable to succeed. We decided to ensure that the hyperparameters we used here would always be adequate by always normalising the data sets we test this technique on.

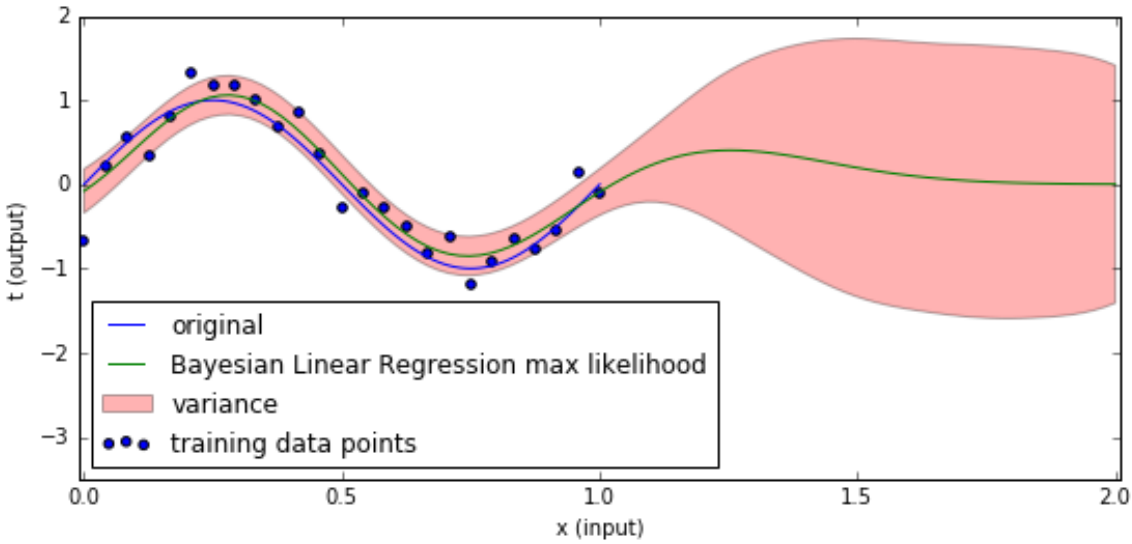

Figure 7: The predictive disribution for linear regression for for the training points shown. The green line shown the mean, or peak, of the probability distribution of the prediction. The boundaries of the pink band show the variance.

3.3.2. Two-Dimensional Synthetic Data

Here we show how we used the predictive distribution method for linear regression and apply it to a synthetic data set with two inputs. We did this to see how well the method holds up when using a more complicated data set. This was also done so that we could have visual confirmation that the algorithm works when using a data set with multiple inputs

We arbitrarily defined a synthetic data that will be suitable for our demonstration. It is shown in figure 8. It is defined by the sum of three different two-dimensional Gaussian distributions. In the figure, warmer colours correspond to larger output values with the peaks having values of about one. Colder colours correspond to lower output values, with the lowest at zero.

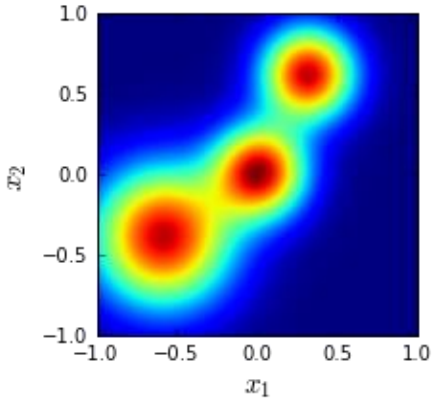

Figure 8: Arbitrarily defined synthetic data with a two-dimensional input, used for demonstrating the predictive distribution in this subsection. It is defined by the sum of three different two-dimensional Gaussian distributions. Warmer colours correspond to larger output values. The range of values is the interval [0, 1].

We generated random training points by uniformly randomly selecting values in the interval [-1, 1] for both of the input dimensions. The points are shown in figure 9.

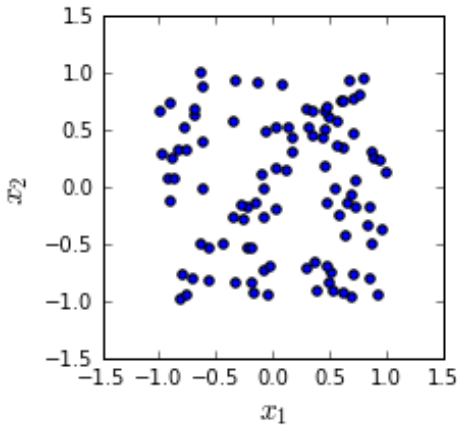

Figure 9: The random training points used in for the demonstration in this subsection.

The means of the Gaussian basis functions for each input dimension has to be chosen so that it corresponds to the mean and variance of the training points' location on that dimension. Alternatively, the training data can be normalised so that for each input dimension, it has a mean of zero and a variance of 0.5. In this study we opted to do the latter. The means and variances of the dimensions of the two-dimensional synthetic data set used in this subsection are already close to these specifications, so in this case it is not necessary to apply the normalization. For most real-life data sets, it will definitely be necessary.

Here we define means for the basis functions we will use for the demonstration in this subsection. If we would use, say, nine Gaussian basis functions for the one-dimensional case, then for an N-dimensional input space, there needs to 9^N basis functions. Their means must be evenly spaced throughout the normalised input space. Since the data set has two dimensions, it will have $9^2 = 81$ basis functions. The means of these basis functions are plotted in figure 10. Since all the input dimensions have more or less the same variance as the input dimension in the demonstration of this technique for data with one-dimensional input, we initially proceeded to continue to use 0.2, 1, and 5 as the values of σ, α, and β respectively.

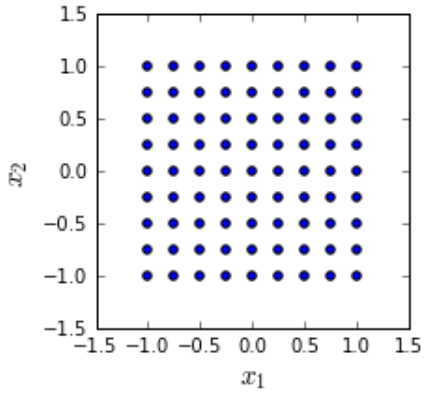

Figure 10: The means of the multivariate Gaussian basis functions used for the demonstration in this subsection.

We defined a test data set consisting of ten thousand points corresponding to a two-dimensional lattice of input points arranged a grid similar to the one shown in figure 10. We define it like this so that we can use the predicted output values that will be yielded as pixels in a heat map image.

We proceeded to use our software to evaluate equations (4) - (8) in python just as we did for the data with a one-dimensional input. We fixed problems with the code that was not apparent when there was only one input dimension. The predicted means is shown as a heat map image in figure 11.

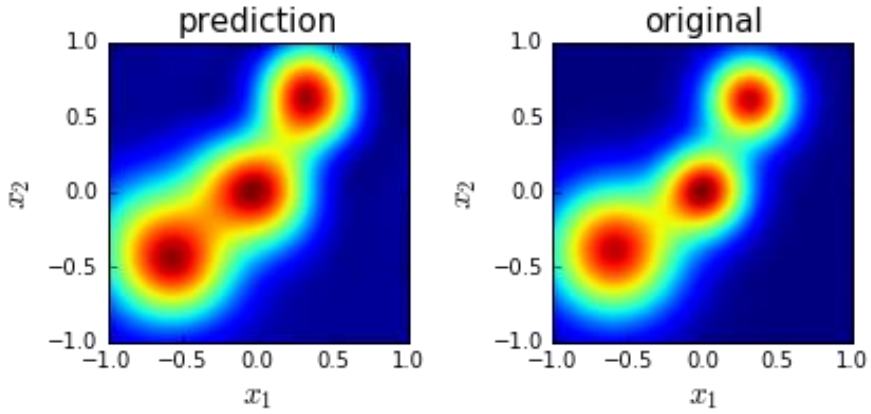

Figure 11: The predictive distribution for linear regression (left) of 10'000 test points representing the 100x100 pixel array in figure 8 (reproduced on the right). Here the values of M, σ, α, and β are 9, 0.2, 1, and 5 respectively. The distribution that the training points were taken from is shown on the right for easy comparison.

As can be seen in the figure the prediction method does indeed hold up for this more complicated data set. The increased size of the data set and the large number of basis functions caused the computations to take a noticeable duration of time, namely a few seconds. This will exponentially increase as the number of dimensions and basis functions increase. We tested the effects of using fewer basis functions, specifically basis functions whose means are a 5x5 grid. The results were greatly inferior, showing us that it is indeed necessary to use as many basis functions as we did.

We investigated the effects that varying the values of σ, α, and β have on the result shown in figure 11. As expected, changing the value of σ caused the plot of the prediction to sharpen or blur with the prediction error to increase accordingly. This was unaffected by a change in the value of M, unlike what one might suspect. However, we did find that the accuracy of the prediction improves significantly with when the value of α is decreased. We found that decreasing its value to something in the order of 0.001 gets the best results in this scenario. The predictive distribution destabilises if α gets much smaller than that.

Using this value for α, we investigated the effect that different values of M have on the accuracy and the calculation time. This is shown in figure 12. The figure also shows the variance of the error, which gives one an indication of how overfit the model is. In this case the overfitting is acceptably low, as evidenced by the correlation between the average error and the error variance.

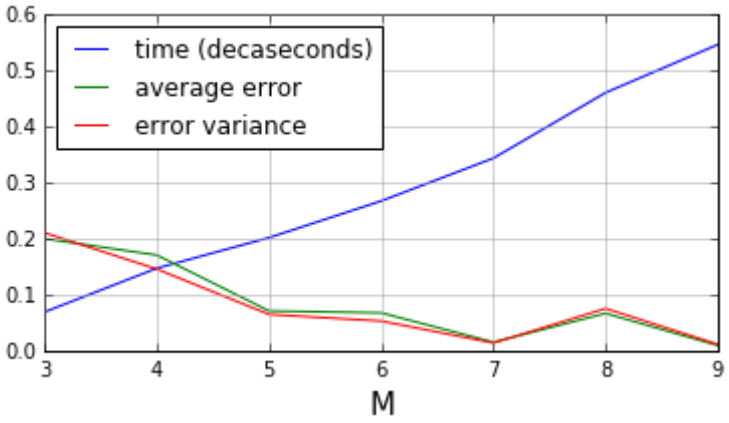

Figure 12: The calculation time, average error, and error variance of the predictive distribution for linear regression with different values of M. The random training points in figure 9 were used as the training points and the test points were 10'000 points representing the 100x100 pixel array in figure 8.

Having thus confirmed that the code works correctly on this synthetic data set, we then proceeded to test it on real world data sets. The data sets this method gets used on should not have many dimensions or the algorithm's computation time will be too long. For example, just setting up basis function means (for M=9) for data with 9 or more dimensions requires more memory than the average computer has.

3.3.3. Real World Data Sets

In this subsection we evaluate the method's performance when tested on real world data sets. The code used for each evaluation is provided in appendix D.

3.3.3.1. Wine Quality

We decided to try the method with a wine quality data set. It has eleven input dimensions and 1'599 entries. Its input dimensions are the properties of a wine product. Its output is a rating out of ten for that product.

It was here that we realised the problem of having too many input dimensions and decided to use only five of the attributes so that not too much computation is needed. In order to reduce computation time further, we limited the number of basis functions 5^5. We normalised the data to have a zero mean and a variance of 0.5. The necessity of this was explained in the previous section. We shuffled the entries of the data set beforehand to ensure that any possible ordering that may have been present in the data set is now non-existent.

We calculated the prediction just as we did before, using the same values of σ, α, and β. The first 1'000 data set entries were used as the training set and the remainder were used as the test points. Despite the limitations, the prediction took about a minute to be computed. In

addition, the limitations had a price. The average of the predicted ratings was 4.61 but the actual ratings are 5.70. The mean predictions deviate from the actual value by an average of 11%.

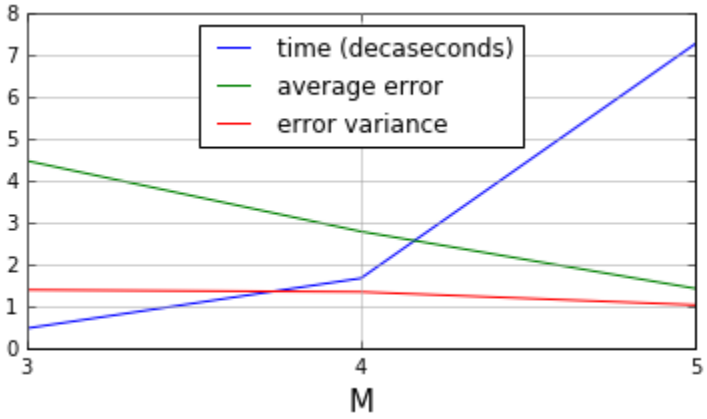

Figure 13: The calculation time, average error, and error variance of the predictive distribution for linear regression with different values of M. A thousand different entries from the wine quality data set were randomly selected and used as the training points. The remaining 599 entries were used as the test points.

We decided to do further tests with this method only on data sets with a small number of dimensions.

3.3.3.2. Weather

Here follows another demonstration of predictive distribution for linear regression. Here we use a climate data set. The attributes of this data set are the date, minimum temperature, maximum temperature, and precipitation for every day of one year. We let the input space be the date, the minimum temperature, and the maximum temperature of a weather station. The precipitation was assigned to be the output.

We normalised the data and used every second entry as the training points. All the samples were used be the test data. The results of using various values of M are shown in figure 14. As expected, the computation time increases with larger values of M. As can be seen in figure 14 the accuracy of the prediction improves with more basis functions. Since the output data in this data set is only specific to the integer and ranges from one to fourteen, we can consider this prediction satisfactory.

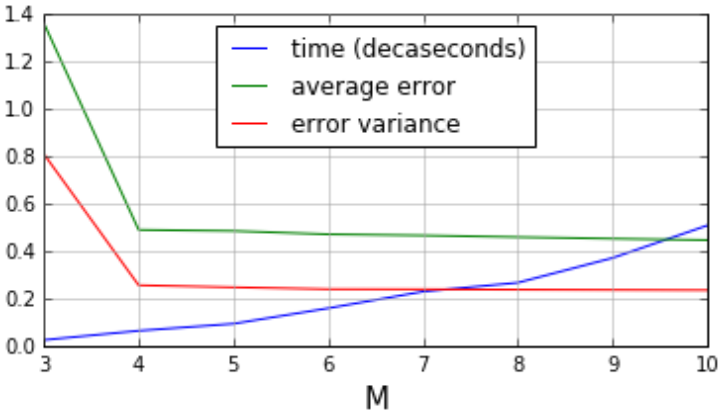

Figure 14: The calculation time, average error, and error variance of the predictive distribution for linear regression with different values of M. Every second entry from the weather data set was used as a training point. All 365 points in the data set were used as test points.

4. Kernel Regression

4.1.Introduction

When using kernel regression, usage is made of the kernel function k(**x**, **x**') that relates any two points on the input space. A Gram matrix **K**, whose elements are given k($\mathbf{x}_n$, $\mathbf{x}_m$), can be defined to relate each possible pairing of two input vectors. These kernel functions can be constructed from previously defined basis functions, like those used for linear regression. Since the basis functions has to be defined first in order to construct the Gram matrix in this way, any new prediction methods that uses the Gram Matrix will also be subjected to the same problematic restrictions that linear regression has. The restriction is that the number of basis functions needed is M^D. M is the number of basis functions that has to be defined for the variation of one input variable while all the other input variables are held constant.

A solution to this problem is to define kernel functions without involving basis functions. There are prerequisites which have to be satisfied when doing so. The Gram matrix has to be a positive semi-definite matrix.

4.2.Nadaraya-Watson Model

Here we show how we attempted to replicate figure 6.3 in Bishop. In this example, the Nadaraya-Watson model is used to evaluate the output of the test input points using equation (9).

$$p(t|x) = \frac{\sum_n f(\mathbf{x} - \mathbf{x}_n, t - t_n)}{\sum_m \int f(\mathbf{x} - \mathbf{x}_m, t - t_m) dt} \tag{9}$$

f(x, t) is a zero-mean isotropic Gaussian with variance σ. m and n are any integers in the interval [0, N-1], where N is the number of training points. The input of the training points are evenly spaced points over the input space interval [0, 1] and the output is a sinusoid with Gaussian noise. It is plotted in figure 15.

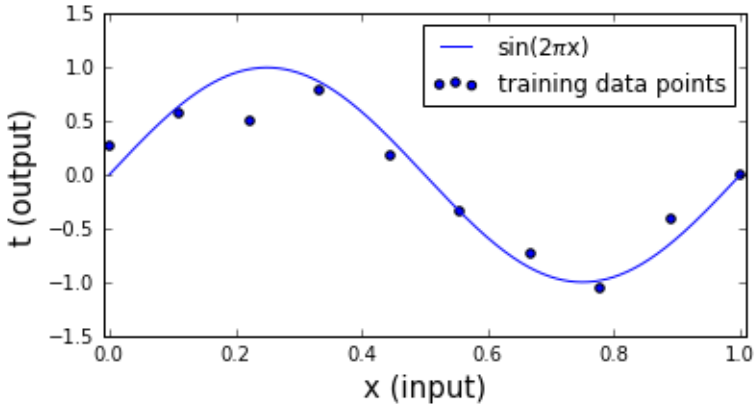

Figure 15: The training data points used for the demonstration of the Nadaraya-Watson model.

The equation for the best prediction is the same as equation (9), except that the *t* argument of f(x, t) is always zero and thus can be ignored. The integral becomes obsolete (equal to one) because its argument no longer contains the *t* variable. We are thus left with equation (10).

$$y(\mathbf{x}) = \frac{\sum_n g(\mathbf{x} - \mathbf{x}_n) t_n}{\sum_m g(\mathbf{x} - \mathbf{x}_m)} \tag{10}$$

The g(x) is the same as the f(x) of before except that the multivariate Gaussian with variance is now only over the input space.

We implemented the code necessary to calculate equation (10) in python. Below is the plot of the prediction after experimenting with different values of σ until one that works well (σ = 0.1) was found.

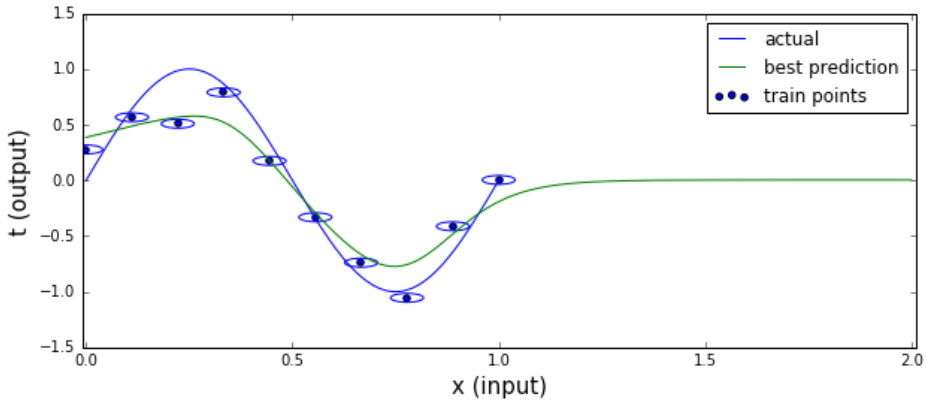

Figure 16: The prediction made by the Nadaraya-Watson model for the training points shown.

We also tried this technique on synthetic data with a two-dimensional input. We used the same arbitrary data set we used for linear regression. It is shown in figure 17.

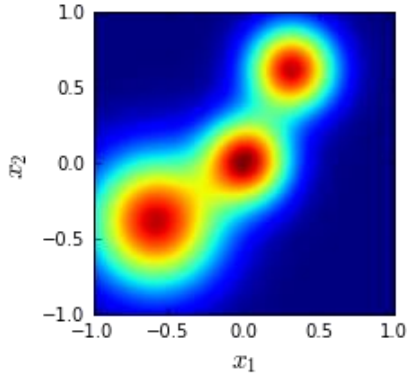

Figure 17: An arbitrary data set with a two-dimensional input, used for the illustration of the Nadaraya-Watson model.

Points on the input space were uniformly randomly selected over the intervals x_1 = [-1, 1] and x_2 = [-1, 1]. These points are plotted in figure 18.

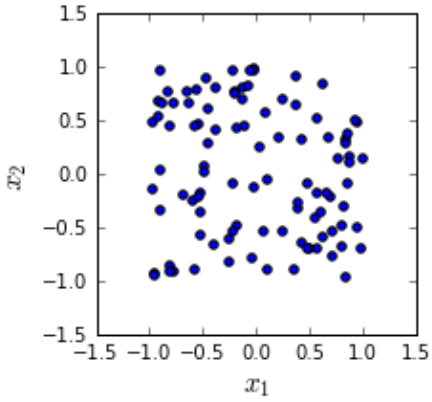

Figure 18: The training points used in for the demonstration in this subsection.

The most likely prediction made by the Nadaraya-Watson model using these training points is shown in the figure 19. The prediction is not very good and is very dependent on my choice of σ. Worse yet, it took several seconds to be computed.

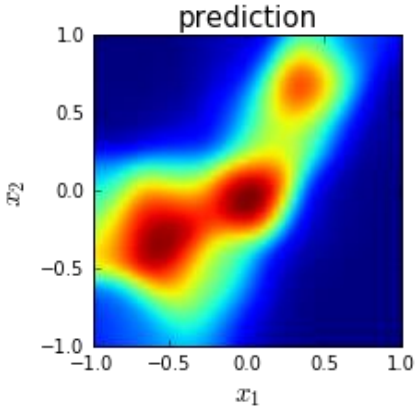

Figure 19: The prediction made using the Nadaraya-Watson model fitted with the training poins in figure 18.

4.3.Gaussian Processes for Regression

Here follows an explanation of Gaussian process for kernel regression. Most of the equations used in this chapter are taken from Bishop's book [Bishop, 2006]. If input values x_1 ,..., x_N and corresponding target values $t_N = (t_1, ..., t_N)^T$ are provided, it can be used to predict the target value t_{N+1} separately for each of the given input values. The given input value for which a prediction is currently being made will be denoted x_{N+1}.

One widely used kernel function for Gaussian processes for kernel regression is given by

$$k(\mathbf{x}_n, \mathbf{x}_m) = \theta_0 exp\{-\frac{\theta_1}{2}||\mathbf{x}_n - \mathbf{x}_m||^2\} + \theta_2 + \theta_3 \mathbf{x}_n^T \mathbf{x}_m \tag{11}$$

where θ_0,...., θ_3 are parameters.

C_{N+1} is an (N+1) × (N+1) covariance matrix with elements given by

$$C(\mathbf{x}_n, \mathbf{x}_m) = k(\mathbf{x}_n, \mathbf{x}_m) + \beta^{-1}\delta_{nm} \tag{12}$$

δ_{nm} is the Dirac delta function, *n* is the row number, and *m* is the column number, which is zero when n and m are equal. The second term of the equation above is thus nonzero only for the main diagonal of C_{N+1}.

C_{N+1} can be partitioned into four different sections, each with their own notation as shown in equation (15). The following two equations can be derived from an analysis of conditional Gaussian distributions.

$$\mu_{a|b} = \mu_a + \Sigma_{ab}\Sigma_{bb}^{-1}(x_b - \mu_b) \tag{13}$$

$$\Sigma_{a|b} = \Sigma_{aa} + \Sigma_{ab}\Sigma_{bb}^{-1}\Sigma_{ba} \tag{14}$$

These equations can then be used to derive equations (16) and (17). These last two equations are the mean and variance of the prediction made by Gaussian processes for kernel regression.

$$C_{N+1} = \begin{pmatrix} C_N & \mathbf{k} \\ \mathbf{k}^T & c \end{pmatrix} \tag{15}$$

$$m(\mathbf{x}_{N+1}) = \mathbf{k}^T C_N^{-1}\mathbf{t} \tag{16}$$

$$\sigma^2(\mathbf{x}_{N+1}) = c - \mathbf{k}^T \mathbf{C}_N^{-1} \mathbf{k} \tag{17}$$

4.3.1. One-Dimensional Synthetic Data

Here follows a demonstration of Gaussian processes for kernel regression for a simple example. As usual, samples of a sinusoid with Gaussian noise were used as training points.

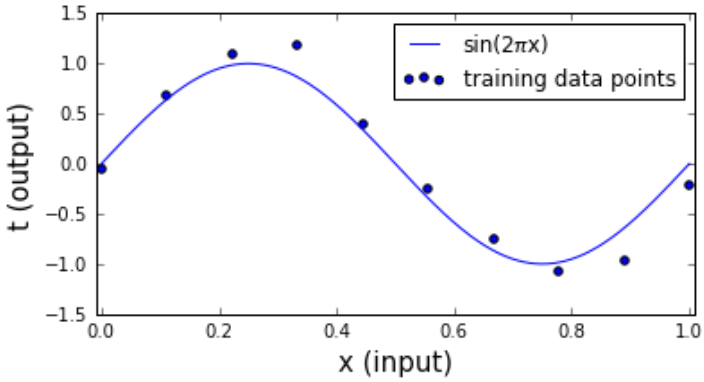

Figure 20: The training points used for the demonstration of a Gaussian processes for kernel regression.

After some experimentation and examining the Bishop's examples, we intuitively decided to initially use 1, 1, 5, and 1 as the respective initial values of the θ parameters. We found that the higher values of β have the effect of decreasing the variance of the prediction. These parameters values and the aforementioned training points were to evaluate $k(x_n, x_m)$. This was then used to calculate C_{N+1}, which was in turn used to predict the mean and variance of the output for inputs over the interval [0, -2]. The results are displayed in figure 21.

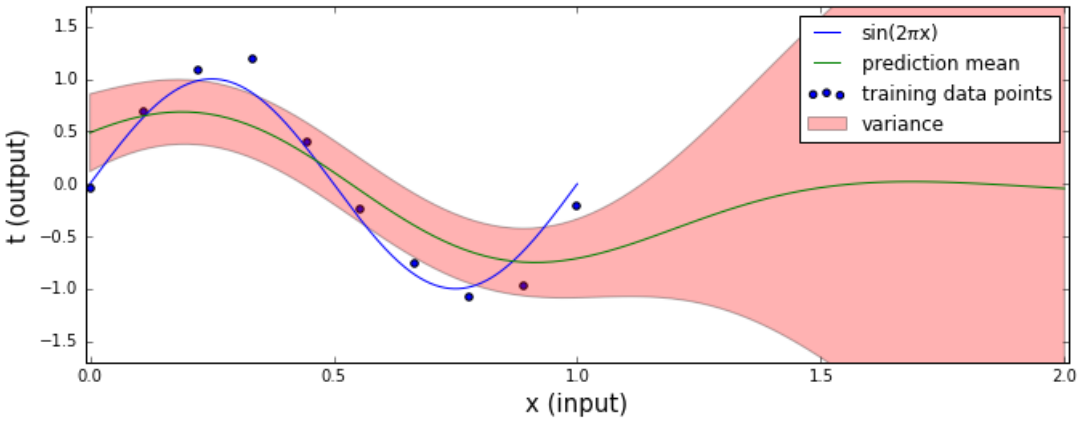

Figure 21: The training point and predictions made using Gaussian processes for kernel regression with selected parameter values.

The result is not satisfactory even after carefully selecting parameter values and thus this technique as described thus far has hardly any practical use. There exists a solution to this predicament. Bishop describes a way of calculating the probability gradient for each parameter value, which can then be used to find better values for the parameters. The equation for determining this is given below.

$$\frac{d}{d\theta_i}\ln p(\mathbf{t}|\theta) = -\frac{1}{2}Tr(C_N^{-1}\frac{dC_N}{d\theta_i}) + \frac{1}{2}\mathbf{t}^T C_N^{-1}\frac{dC_N}{d\theta_i}C_N^{-1}\mathbf{t} \tag{18}$$

The 'i' variable can take on positive integer values up to the number parameters in the kernel function that is being used in this method. The one we used has four parameters. In order to evaluate equation (18), we determined expressions for the derivative term on the right-hand side of that equation. The equations for evaluating that derivative term for each of the four parameters are given below.

$$\frac{dC_N}{d\theta_0} = exp\{-\frac{\theta_1}{2}||\mathsf{x}_n - \mathsf{x}_m||^2\} \tag{19}$$

$$\frac{dC_N}{d\theta_1} = \theta_0(exp\{-\frac{\theta_1}{2}||\mathsf{x}_n - \mathsf{x}_m||^2\})\{-\frac{1}{2}||\mathsf{x}_n - \mathsf{x}_m||^2\} \tag{20}$$

$$\frac{dC_N}{d\theta_2} = 1 \tag{21}$$

$$\frac{dC_N}{d\theta_3} = \mathsf{x}_n^T\mathsf{x}_m \tag{22}$$

Python code was written to evaluate equations (19) to (22). We used the same aforementioned values of the parameters as prior values for calculating the equation. After they were all calculated, we subtracted the value of the equation for each parameter from the respective parameter. We found that the new values of the parameters causes the regression algorithm to make better predictions. We repeated this process 20 times. The values of the parameters over the course of these iterations are shown in figure 22.

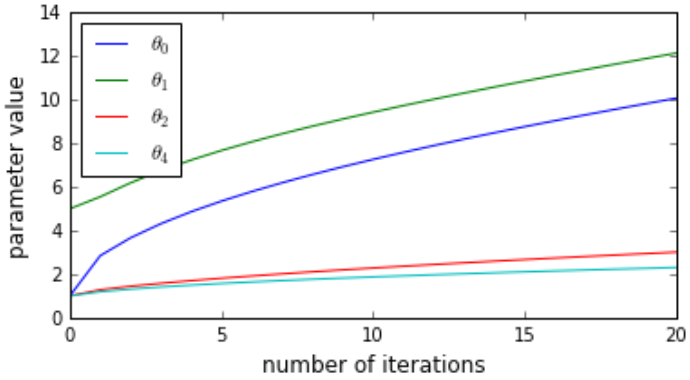

Figure 22: The values of the parameters of equation (11) after repeatedly subtracted the value of equation (18) for each parameter, and then subtracting it from that parameter. The training points in figure 20 were used for the evaluation of these equations. The values of the parameters at zero on the iteration axis are the arbitrarily prior values of the parameters chosen before iterations of the optimization.

Figure 23 shows the prediction using the parameters obtained after 20 iterations. This is good prediction.

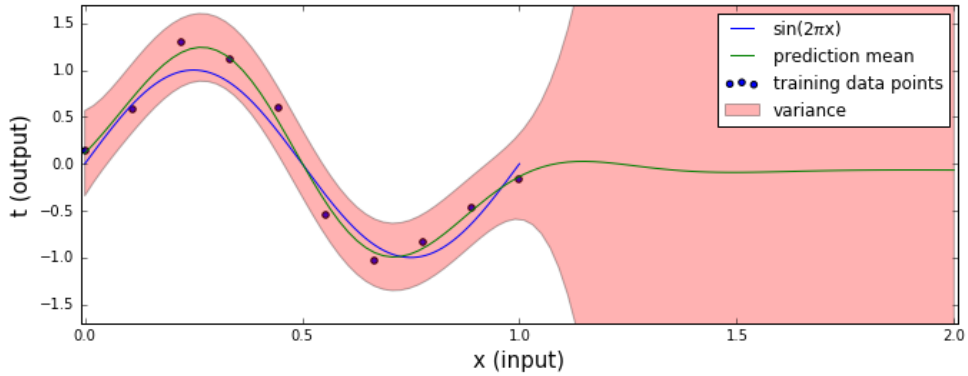

Figure 23: The results of using Gaussian processes for kernel regression after twenty iterations of optimization.

Using very many iterations or choosing very high prior parameters yields the problematic result in figure 24.

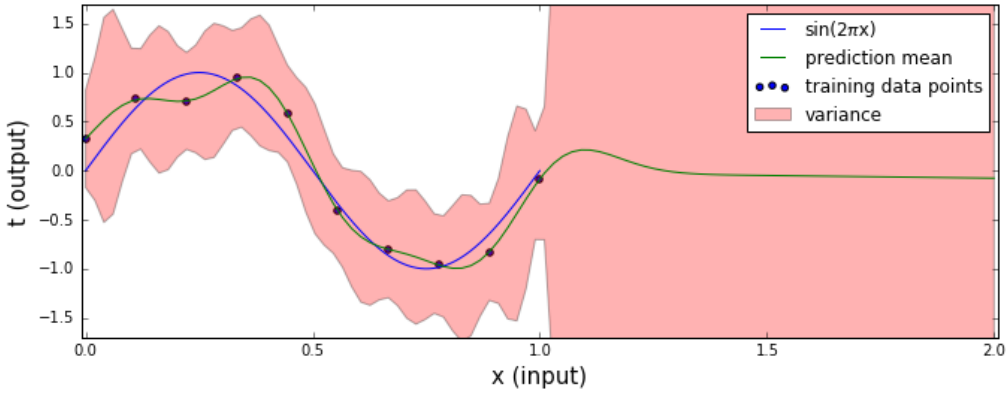

Figure 24: The results of using Gaussian processes for kernel regression after 500 iterations of optimization.

Although all the training points were predicted perfectly, the prediction no longer represents the sinusoidal wave that the training points were derived from. This is an example of what one would call “over fitting”. This technique would thus work very well if the training points are noiseless (unlike this example). Care needs to be taken when applying this parameter estimator.

4.3.2. Two-Dimensional Synthetic Data

Here we show we took Gaussian processes for kernel regression and applied it to synthetic data with a two-dimensional input. We once again used the data set shown in figure 25.

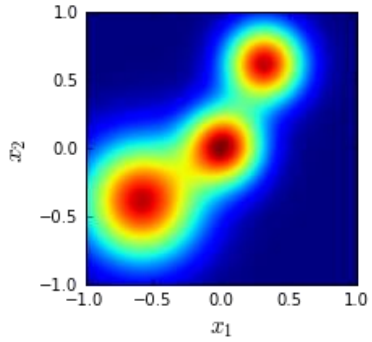

Figure 25: An arbitrarily defined synthetic data set with two inputs.

Again we used one hundred uniformly random points over the intervals x_1 = [-1, 1] and x_2 = [-1, 1], as shown in figure 26.

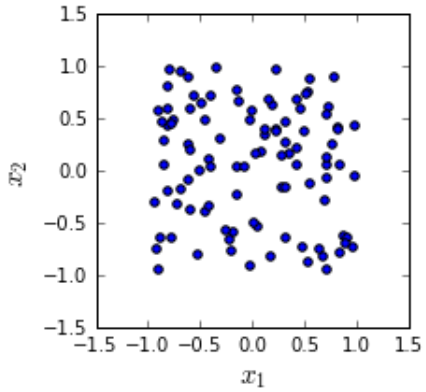

Figure 26: The training points used for the demonstration in this subsection.

In order to prevent the calculations from taking too long, we reduced the number of test points and by extension the resolution of the image render of the result, shown in figure 27.

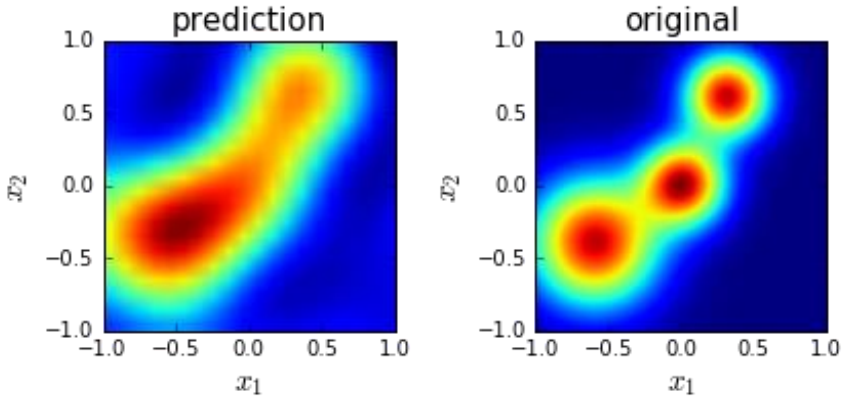

Figure 27: The prediction made by Gaussian processes for kernel regression (left). The distribution that the training points were taken from is shown on the right for easy comparison.

Bishop explains that number of calculations needed for this method is the function $O(N^3)$, where N is number of training points. This is contrary to linear regression, where the computational complexity function is $O(M^3)$ where M is the number of basis functions, which exponentially increases with the number of dimensions. It is thus unfeasible to use linear regression on data sets with large numbers (more than about five) of dimensions. Contrariwise, using Gaussian process for kernel regression is feasible with data sets with a large number of dimensions. Gaussian processes for kernel regression are instead practically limited by the number of training and test points.

We applied optimization just as we did for the one-dimensional data. It was computed very quickly. Figure 28 shows how the parameters changed over twenty iterations of optimization. We used the same prior values of the parameters we used for the one-dimensional case.

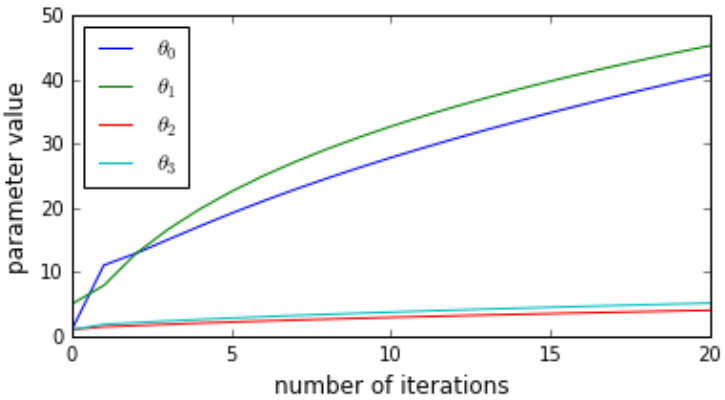

Figure 28: The values of the parameters during the course of twenty iterations of optimization.

Figure 29 shows the result of the predictions made using the parameters yielded after the optimization. Even though the resolution is low, we can still see that the predictions' distributions are fairly accurate.

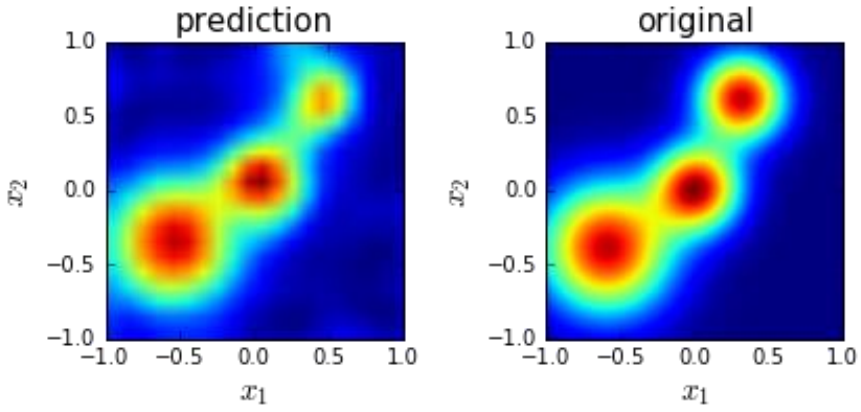

Figure 29: The prediction made by Gaussian processes for kernel regression (left) after twenty iterations of optimization, displayed as a heatmap. Note that the range of the ouput of the picture on the left is a bit smaller than the one on the right. The distribution that the training points were taken from is shown on the right for easy comparison.

We tested with different numbers of training points. It would appear that the calculation time increases quadratically with the number of training points. The accuracy and calculation time that results from using different numbers of iterations of optimisation is shown in figure 30.

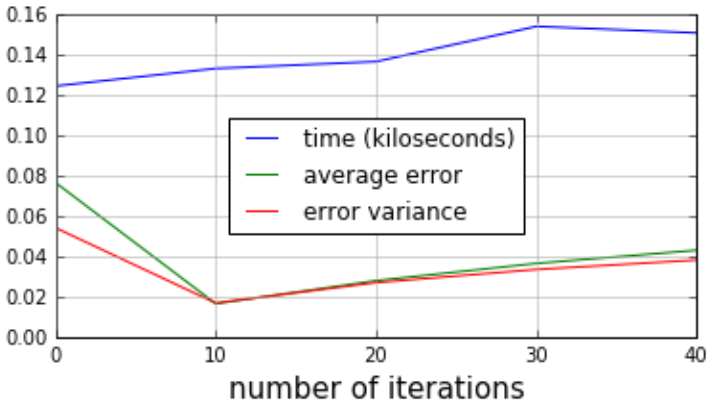

Figure 30: The calculation time, average error, and error variance of Gaussian processes for kernel regression applied to the training points shown in figure 26. The test points were 400 points representing a 20x20 pixel array of the data shown in figure 25.

Since figure 29 shows us that the shape of the predictions' distribution is close to the original, one might think that the prediction can be corrected simply by multiplying the predictions with a constant. This would not be right because, as illustrated in the next subsection, this method predicts the training points accurately. We believe the problem must therefore be that the predictions of the test points that are not close enough to the training points have an undesired decrease in their values.

4.3.3. Real World Data Sets

Here we show how we tested Gaussian processes for kernel regression on real-world data sets. The code used for each evaluation is provided in appendix D.

4.3.3.1. Wine Quality

The first set we used was the same shuffled wine quality data set on which we tested linear regression. We used fifty of the entries as training points and another 500 entries as test points. We made predictions of both the training points and the test points. Figures 31 and 32 show how the computation time, average error, and the average error variance changes for different numbers of optimization iterations. The result of using the same subset of the wine quality data set on both the linear regression method and the kernel regression method is included in appendix C.

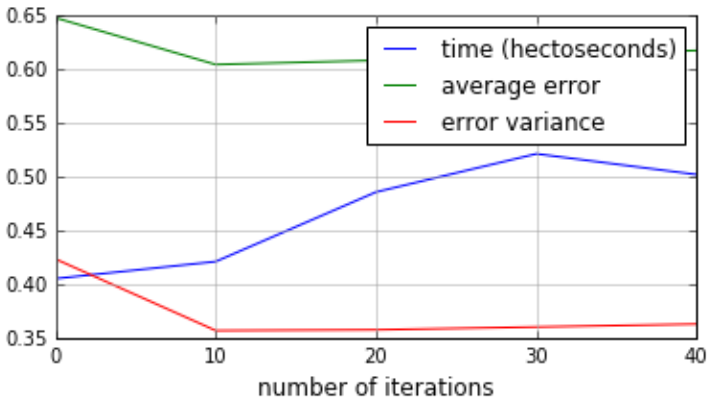

Figure 31: The calculation time, average error, and error variance of Gaussian processes for kernel regression using various numbers of optimization iterations. Fifty different entries from the shuffled wine quality data set were randomly selected and used as the training points. Another fifty entries were used as the test points.

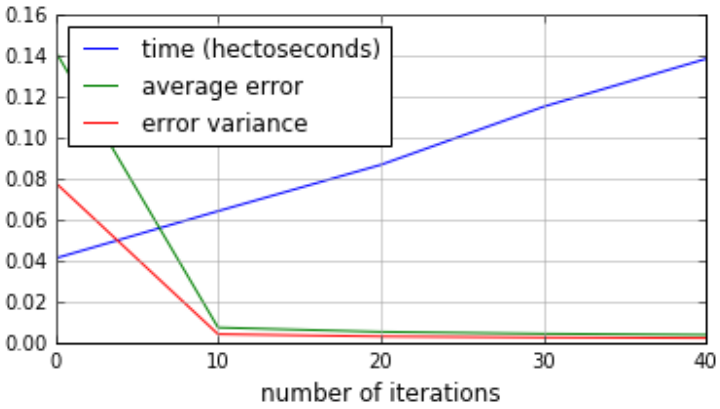

Figure 32: The calculation time, average error, and error variance of Gaussian processes for kernel regression using various numbers of optimization iterations. Fifty different entries from the shuffled wine quality data set were randomly selected and used as the training points. Here these same training points are also used as the test points.

4.3.3.2. Diabetes

We then tested it on a diabetes data set, which has eight inputs and one binary output. This data set has some missing data. We filled each missing data entry with the average of its respective attribute. We calculated the prediction with 100 test points, treating the output as a continuous variable in which the numbers zero and one are assigned to the two classes. We classified each test point according to which binary class the prediction's value was closest. Table 33 shows the results before and after optimization.

Training Points	50	100
Prediction computation time	49	200
number of erroneous classifications before optimization	150	135
number of erroneous classifications after optimization	139	138

Figure 33: The results of using 50 or 100 training points when using Gaussian processes for kernel regression to make predictions based on the diabetes data set.

5. Conclusions

The methods that were tested in this project have limited usefulness as means of prediction. They work best when the input coordinates of the test data occurs in the same general area as that of the training data for each of the input dimensions. The method of using the predictive distribution for linear regression is feasible only when there are a small number of input dimensions. The method of using Gaussian processes for kernel regression, using the provided kernel function, can easily handle data with a large number of dimensions, but becomes unfeasible when the number of training points become large.

We would recommend finding a solution to the unfeasibility problems stated previously. The flaws could be inherent in the methods or it could be a result of the way we implemented it. We also recommend finding methods that can make accurate predictions of test data that is not localised to the training data's general area on the input dimensions.

Appendices

Appendix A: Project Planning Schedule

The project leader and the student met shortly after the project allocations were released. It was agreed on that the student would take time during the June vacation to go through selected pieces of relevant literature. The student would familiarise himself with the content of the literature and identify parts of the literature that contains content that can be of use in this project.

The project leader and the student did not decide that a precise schedule has to be followed. The project progress during the second semester was more or less assigned to the schedule below. The student had to use his own judgment to decide if the sufficient progress has been made.

- First two weeks the first term: Study selected relevant sections in literature.
- Rest of the first term: Write the software necessary to implement linear regression. Test on all the necessary types of data sets and debug as necessary. Make appropriate observations
- Mid-semester break and first two weeks of second term: Write the software necessary to implement kernel-based regression. Test on all the necessary types of data sets and debug as necessary. Make appropriate observations.
- Rest of the second term: Finalise the report. Make changes and additions to previous work as appropriate.

Appendix B: Outcomes Compliance

Problem Solving

It was identified that the problem is there cases that a variable in a system is sometimes unknown while there are other known variables that remain known even when the former variable becomes is no longer known. It was also known that there is no mathematical model which relates the variables to each other. The solution was to make predictions using statistical models to determine the influence the known variables has on the unknown variables.

It was determined that the solution could be realised by consulting relevant literature to find and understand suitable models. Software would then be written to implement these models. These models would then be tested with simple synthetic data to determine how well they work and whether it was implemented correctly. The models would then be tested on real data and the results would be analysed. The implementation of the models and evaluation of the tests made on them is in the body of this report.

Application of Scientific and Engineering Knowledge

The problems were analysed and solutions were presented in a formal manner. The underlying concepts and theories of the solutions are explained in this report. In cases of uncertainty, informed judgments were made. The statistical models in this project have its basis in mathematical definitions that comply with the laws of physics.

The engineering problem that was explored in this project has already been the subject of research. Existing techniques of solving the problem were utilised and evaluated. An ultimate solution has yet to be determined for the problem and there is still room for more research on this topic.

Engineering Design

It was identified that the problem of predicting an unknown value in a system when other values in the system are known. The design process was explained in appendix A. Literature was consulted to acquire requisite knowledge which was then evaluated. The design task of writing the software to perform the desired algorithms was completed and optimised. We evaluated multiple solutions, judging them and comparing them. The report explains the logic behind the design and shows information that influenced it.

Investigations, experiments and data analysis

We planned our investigation by selecting relevant literature and studying to find solutions. We selected and use the Jupyter software in the WinPython package. We gave analyses and made interpretations of the results of our experiments. Conclusions were drawn in chapter 5.

Engineering Methods, Skills and Tools, Including Information Technology

In this project, appropriate regression methods were identified. They were implemented as custom made computer applications. They were tested on data sets in a logical manner. The results are presented with accompanying assessment and critique.

Professional and Technical Communication

The report was written according to the guidelines provided by the engineering faculty in which this study was done. The designs and experiments in this report are effectively illustrated with figures. The underlying mathematics is stated and a list of symbols are provided.

Independent Learning Ability

As previously explained in this report, literature was studied and the acquired knowledge was reflected on. The sources are stated. Different regression methods were assessed and comprehended independently. The acquired knowledge was then used to implement computer programs without formal instruction.

Appendix C: Additional Simulations

Here we include an illustration of how the linear regression method and the kernel regression method compare to each other when used on the same subset of the wine quality data set. Here fifty random entries were used as the training points and another one hundred were used as the test points. Only the first five attributes of the data sets were included. These restrictions were made to ensure that both of the methods functions within limits imposed by technology and time constraints.

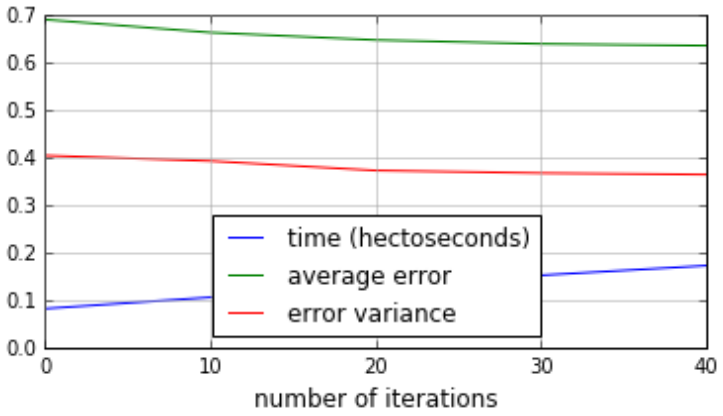

Figure 34: The calculation time, average error, and error variance of the predictive distribution for linear regression with different values of M. Fifty different entries from the wine quality data set were randomly selected and used as the training points. Another one hundred entries were used as test points.

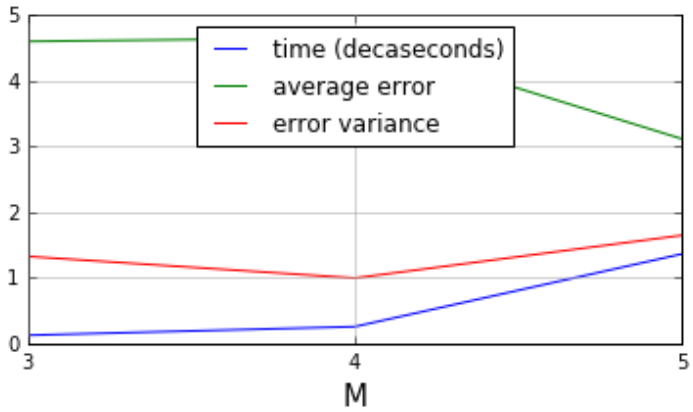

Figure 35: The calculation time, average error, and error variance of Gaussian processes for kernel regression using various numbers of optimization iterations. Fifty different entries from the wine quality data set were randomly selected and used as the training points. Another one hundred entries were used as test points.

Appendix D: Code

The python code for doing both of the regression methods in this project is included below. The predictive distribution for linear regression is done by calling the “lin_reg_pred_distrib” function. Gaussian processes for kernel regression can be done by calling the “Gauss_proc_kern_reg” function. Shown below is the code for these two functions, preceded by all their prerequisite functions. The inputs and outputs of the two functions are explained in their comments.

```
import numpy as np
import pylab as pl
from numpy.linalg import inv
import time

def heatmap_random(data,n):
    #

    w0 = np.zeros(n)
    w1 = np.zeros(n)

    for a in range(0,n):
        data_raveled = data.ravel()
        data_sum = np.sum(data_raveled)
        q = 0
        o = np.random.uniform(0,1) * data_sum
        e = 0
        i=1
        while e==0:
            q += data_raveled[i]
            if (q > o):
                e = i
                break
            i+=1
        w1[a] = -1 + (e/100 - (e%100)/100)*0.02
        w0[a] = -1 + (e%100)*0.02
    return w0, w1

def basis(x,mu,s):
    #the function for evaluating a basis function given a point in N-dimensional input space and also a mean and a variance.
    D = np.shape(mu)[0]
    magnitude = 0
    for a in range(0,D):
        magnitude += (x[a] - mu[a])**2
    magnitude = np.sqrt(magnitude)
    phi = np.exp(-(magnitude**2)/(2*(s**2)))
    return phi

def com_gauss_proc_kern(x_n, x_m, theta0, theta1, theta2, theta3):
    #the name is a shortened form of "common Gaussian process kernel".
    #This function calculates equation 6.63 for given parameters and 2 given x vectors.
    #Note: x_n and x_m has to be arrays. It has to be defined with functions like "np.array" or
    #"np.atleast_2d". Declarations like "x = 1" or "x = [3,3]" will not work.
    #The theta arguments are single values
    x_n = x_n.ravel()
    x_m = x_m.ravel()
    term1 = theta0*np.exp( (-theta1/2)*((np.sqrt( ((np.subtract(x_m,x_n))**2).sum()  ))**2)  )
    result = term1 + theta2 + theta3*np.sum(x_n*x_m)
    return result

def gauss_proc_kern_reg_cov(x_train, x_test, theta0, theta1, theta2, theta3, beta):
    #the name is a shortened form of "Gaussian process kernel regression covariance"
    #x_train is a an (n, d) array, where d is the number of dimensions and n is the number of training points.
    #if x_train is one-dimensional, use np.atleast_2d on it before passing it ti this definition
    #returns: cov_N, k, k_T, c, cov_full, inv_cov_N
    n, d = np.shape(x_train)
    x_full = np.append(x_train,np.atleast_2d(x_test)).reshape(n+1,d)
    cov = np.zeros([n+1,n+1])
    for a in range(0,n+1):
        for b in range(0,n+1):
            cov[a,b] = com_gauss_proc_kern(x_full[a,:], x_full[b,:], theta0, theta1, theta2, theta3 )
            if (a==b):
                cov[a,b] += (1/beta)
    inv_cov_N = inv(cov[:n,:n])
    return cov[:n,:n], cov[:n,n], cov[n,:n], cov[n,n], cov, inv_cov_N

def gauss_proc_kern_reg_pred_mean(k_T,C_N,t, inv_cov_N):
    #the name is a shortened form of "Gaussian process kernel regression prediction mean"
    o = np.dot(k_T,inv_cov_N)
    i = np.dot(np.atleast_2d(o),np.atleast_2d(t.ravel()).transpose() )
    return i

def gauss_proc_kern_reg_pred_var(c,k_T,C_N,k, inv_cov_N):
    #the name is a shortened form of "Gaussian process kernel regression prediction variance"
    o = np.dot(k_T,inv_cov_N)
    i = c - np.dot(np.atleast_2d(o),k )
    return i

def theta0_deriv(x_n, x_m, theta0, theta1):
```

```
    x_n = x_n.ravel()
    x_m = x_m.ravel()
    result = np.exp( (-theta1/2)*((np.sqrt( ((np.subtract(x_m,x_n))**2).sum()  ))**2)  )
    return result
def theta1_deriv(x_n, x_m, theta0, theta1):
    x_n = x_n.ravel()
    x_m = x_m.ravel()
    result1 = theta0*np.exp( (-theta1/2)*((np.sqrt( ((np.subtract(x_m,x_n))**2).sum()  ))**2)  )
    result = result1*(-1/2)*((np.sqrt( ((np.subtract(x_m,x_n))**2).sum()  ))**2)
    return result
def theta3_deriv(x_n, x_m, theta3):
    x_n = x_n.ravel()
    x_m = x_m.ravel()
    result = np.sum(x_n*x_m)
    return result

def gauss_proc_kern_reg_deriv_values(x_train, theta0, theta1, theta2, theta3, beta):
    #the name is a shortened form of "Gaussian process kernel regression derivative values"
    #It returns all the values needed to solve equation (6.70)
    #x_train is a an (n, d) array, where d is the number of dimensions and n is the number of training points.
    #if x_train is one-dimensional, use np.atleast_2d on it before passing it ti this definition
    #returns: cov_N, k, k_T, c, cov_full
    n, d = np.shape(x_train)
    cov = np.zeros([n,n])
    cov_theta0_deriv = np.zeros([n,n])
    cov_theta1_deriv = np.zeros([n,n])
    cov_theta2_deriv = np.zeros([n,n])
    cov_theta3_deriv = np.zeros([n,n])
    for a in range(0,n):
        for b in range(0,n):
            cov[a,b] = com_gauss_proc_kern(x_train[a,:], x_train[b,:], theta0, theta1, theta2, theta3 )
            cov_theta0_deriv[a,b] = theta0_deriv(x_train[a,:], x_train[b,:], theta0, theta1 )
            cov_theta1_deriv[a,b] = theta1_deriv(x_train[a,:], x_train[b,:], theta0, theta1 )
            cov_theta2_deriv[a,b] = 1
            cov_theta3_deriv[a,b] = theta3_deriv(x_train[a,:], x_train[b,:], theta3 )
            if (a==b):
                cov[a,b] += (1/beta)
    inv_cov = inv(cov) #inverse of the matrix covariance
    return cov, inv_cov, cov_theta0_deriv, cov_theta1_deriv, cov_theta2_deriv, cov_theta3_deriv

def gauss_proc_kern_reg_deriv(x_train, t_train, inv_cov, cov_theta_deriv):
    #Implementation of equation 6.70 in [Bishop, 2006]
    term1 = (-1/2)*np.trace(np.dot(inv_cov,cov_theta_deriv))
    term2 = np.dot(t_train.transpose(),inv_cov)
    term2 = np.dot(term2,cov_theta_deriv)
    term2 = np.dot(term2,inv_cov)
    term2 = (1/2)*np.dot(term2,t_train)
    result = term1 + term2
    return result
def optim_kern_param(theta0,theta1,theta2,theta3,beta,N,x_train,t_train):
    #optmise kernel parameters
    #for the specified kernel (Bishop equation 6.63)

    #arrays to hold the values of the parameters after each iteration
    theta0_array = [theta0]
    theta1_array = [theta1]
    theta2_array = [theta2]
    theta3_array = [theta3]

    #variables to hold the value of the parameters after each iteration. They are initially given the prior values.
    theta0_new = theta0
    theta1_new = theta1
    theta2_new = theta2
    theta3_new = theta3

    for a in range(0,N):
        q,w,e,r,t,y = gauss_proc_kern_reg_deriv_values(x_train, theta0_new, theta1_new, theta2_new, theta3_new, beta)
        cov = q
        inv_cov = w
        cov_theta0_deriv = e
        cov_theta1_deriv = r
        cov_theta2_deriv = t
        cov_theta3_deriv = y
        theta0_grad = gauss_proc_kern_reg_deriv(x_train, t_train, inv_cov, cov_theta0_deriv)
        theta1_grad = gauss_proc_kern_reg_deriv(x_train, t_train, inv_cov, cov_theta1_deriv)
        theta2_grad = gauss_proc_kern_reg_deriv(x_train, t_train, inv_cov, cov_theta2_deriv)
        theta3_grad = gauss_proc_kern_reg_deriv(x_train, t_train, inv_cov, cov_theta3_deriv)
        theta0_new -= theta0_grad
        theta1_new -= theta1_grad
        theta2_new -= theta2_grad
        theta3_new -= theta3_grad
        theta0_array = np.append(theta0_array,theta0_new)
        theta1_array = np.append(theta1_array,theta1_new)
        theta2_array = np.append(theta2_array,theta2_new)
        theta3_array = np.append(theta3_array,theta3_new)

    return theta0_new,theta1_new,theta2_new,theta3_new,theta0_array,theta1_array,theta2_array,theta3_array

def lin_reg_pred_distrib(train_x,train_y,test_x,test_y,M,alpha,beta,s):
    #Linear regression predictive distribution
    #inputs:
    # train_x: the input of the training data
    # train_y: the output of the training data
    # test_x: the input of the test data
    # test_x: the output of the test data
    # M: basis function ticks for each dimension (i.e. M^D basis functions)
    # alpha: hyperparameter
    # beta: hyperparameter
    # s: the variance of the Gaussian basis functions
    #outputs:
    # pred_means: an array of the mean of the prediction for each test point
    # pred_means: the average of pred_means
    # test_pred_avg_error: the average error of the prediction
```

```
    # test_pred_error_vari: the variance of test_pred_avg_error
    # calc_time: the time the this definition took to run.

    D = np.shape(train_x)[1]

    c1 = time.process_time()

    means = np.zeros((M**D,D))
    done = 0
    mu_vector_amount = M**D
    row_count = 0
    column_count = 0
    for a in range(0,mu_vector_amount*D):
        means[row_count,column_count] = ( (row_count//(M**column_count))%M*2/(M-1)) - 1
        row_count += 1
        if (row_count == mu_vector_amount):
            row_count = 0
            column_count += 1

    design_matrix = np.zeros((np.shape(train_x)[0],M**D))
    for a in range(0,M**D):
        for b in range(0,np.shape(train_x)[0]):
            design_matrix[b,a] = basis(train_x[b,:],means[a,:],s)
    S_N = inv( alpha*(np.identity(M**D)) + beta*np.dot(design_matrix.transpose(),design_matrix) )
    m_N = beta * (   np.dot( np.dot(S_N,design_matrix.transpose()), np.atleast_2d(train_y).transpose() ) )

    pred_means = np.zeros(np.shape(test_x)[0])
    for b in range(0,np.shape(test_x)[0]):

        phi_vector_pred = np.zeros(M**D)
        for a in range(0,M**D):
            phi_vector_pred[a] = basis(test_x[b,:],means[a],s)
        phi_vector_pred = np.atleast_2d(phi_vector_pred).transpose()

        pred_means[b] = np.dot( m_N.transpose(), phi_vector_pred )

    c2 = time.process_time()
    calc_time = c2 - c1

    pred_means_avg = np.average(pred_means)

    #test_y = test_y.reshape(100,100).transpose()
    #test_y = test_y.ravel()

    test_pred_error = np.abs(pred_means-test_y)
    test_pred_avg_error = np.average(test_pred_error)

    test_pred_error_dev = np.abs(test_pred_error - test_pred_avg_error)
    test_pred_error_vari = np.average(test_pred_error_dev)

    return pred_means, pred_means_avg, test_pred_avg_error, test_pred_error_vari, calc_time


def Gauss_proc_kern_reg(train_x,train_y,test_x,test_y,N,beta,theta0,theta1,theta2,theta3):
    #Gaussian process kernel regression
    #inputs:
    # train_x: the input of the training data
    # train_y: the output of the training data
    # test_x: the input of the test data
    # test_x: the output of the test data
    # N: number of iterations of optimisation
    # beta: parameter
    # theta0: parameter
    # theta1: parameter
    # theta2: parameter
    # theta3: parameter
    #outputs:
    # pred_means: an array of the mean of the prediction for each test point
    # pred_means: the average of pred_means
    # test_pred_avg_error: the average error of the prediction
    # test_pred_error_vari: the variance of test_pred_avg_error
    # calc_time: the time the this definition took to run.

    c1 = time.process_time()

    N_train = np.shape(test_y)[0]

    e1,e2,e3,e4,e5,e6,e7,e8 = optim_kern_param(theta0,theta1,theta2,theta3,beta,N,train_x,train_y)
    theta0 = e1; theta1 = e2; theta2 = e3; theta3 = e4
    theta0_array = e5; theta1_array = e6; theta2_array = e7; theta3_array = e8

    pred_means = np.zeros(N_train)
    pred_vars = np.zeros(N_train)
    for a in range(0,N_train):
        C_N, k, k_T, c, C_N_full, inv_cov_N = gauss_proc_kern_reg_cov(train_x,test_x[a,:],theta0,theta1,theta2,theta3,beta)
        pred_means[a] = gauss_proc_kern_reg_pred_mean(k_T,C_N,train_y, inv_cov_N)
        pred_vars[a] = gauss_proc_kern_reg_pred_var(c,k_T,C_N,k, inv_cov_N)

    c2 = time.process_time()
    calc_time = c2 - c1

    pred_means_avg = np.average(pred_means)

    test_pred_error = np.abs(pred_means-test_y)
    test_pred_avg_error = np.average(test_pred_error)

    test_pred_error_dev = np.abs(test_pred_error - test_pred_avg_error)
    test_pred_error_vari = np.average(test_pred_error_dev)

    return pred_means, pred_means_avg, test_pred_avg_error, test_pred_error_vari, calc_time
```

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