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Computational Complexity and Training Time Synthesis of Gaussian Process Regression Kernels for Monthly Rainfall Intensity Estimation

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Abstract: The precise forecasting of monthly rainfall intensity has been considered as one of the most vital topics in hydrological and climatology studies. Gaussian Process Regression (GPR) has recently emerged as a powerful non-parametric approach to machine learning capable of solving such problems. The choice of covariance function, or kernel, has some impact on the precision of the predictions and computing resources. In this paper, we will discuss how nine widely used GPR kernels, such as Matérn kernels 32 and 52, Exponential, Rational Quadratic kernels and others, affect the effectiveness and computational complexity of modeling of the approximation mapping for monthly rainfall intensity datasets. Our study has found that the optimal efficiency can be reached with the use of the following mixed kernels: ArdExponential, ArdMatérn32 and ArdMatern52 kernels. The obtained optimal efficiency can be explained by the higher suitability of such kernels regarding the intermittent behaviour of precipitation properties compared to other types of kernels. As a result, the use of the mentioned mixture kernels, namely ArdExponential, ArdMatérn32 and ArdMatern52 kernels, allows for achieving high-precision predictions while retaining efficient model architecture.

Keywords: GPR Machine learning, Mixture Kernels, Rainfall intensity, Computational cost, Computational efficiency.

1. Introduction

The accurate mapping approximation of monthly rainfall intensities continues to be among the most critical concerns in hydrologic engineering and regional climatic studies (Ojuh and Joseph, 2021). Precise forecasts are required in order to develop sound measures in managing water resources, planning for agriculture operations and minimizing the chances of flooding disasters (Ibrahim et al, 2022, Akhirevbulu, 2026a).

In recent times, Gaussian Process Regression (GPR) has grown to become one of the fundamental building blocks of modern statistical modeling and machine learning systems, appreciated primarily for its flexible Bayesian approach. In contrast to conventional parametric methods that fit the data into a predefined model structure, GPR uses an entirely different approach and works with an ensemble of models defined via a function distribution that enables the data to speak for itself. The power of such an approach lies in the fact that apart from providing a predictive result, it also offers a natural way of estimating uncertainty associated with each prediction. In other words, GPR gives the mean value for every prediction along with the estimate of variance which allows assessing how much is known about the predicted results. Such a capability is extremely useful for high-risk areas, including climate modeling, financial predictions, and robotics process control, as knowing how reliable a particular prediction is becomes crucial at those points. Moreover, by making use of covariance, which is calculated based on a kernel, GPR finds the optimal balance between bias and variance.

Nevertheless, the performance of a Gaussian process regression model depends on the kernel selected because it defines the basic mathematical foundation for the operation. The kernel makes assumptions about the degree of smoothness, periodicity and correlation in the data, thereby making it a significant factor in how efficient the model will perform in terms of predicting future values, generalizing the model to new climate data and reducing the computing complexity in training the model (Isabona and Ojuh, 2021).

The focus of Akhirevbulu, 2026b, was on geophysics predictive modelling review using machine leaning tools. In this paper, a thorough comparative analysis of the effect of nine different covariance functions on the modelling of monthly rainfall data is presented. The Matérn family of kernels, namely Matérn 32 and Matérn 52, which offer differentiable smoothness for modelling the non-stationary nature of rainfall data; the Exponential kernel, also known as the Ornstein–Uhlenbeck process; the Rational Quadratic kernel, and finally five other kernel types are all considered for different aspects of the time-based variance.

Besides accuracy, the study explores the underlying computational difficulties in the design of GPR models. In particular, the focus is on the O (N^3) complexity of the inverse operation of the matrix in the training step and its influence on hyper-parameter optimisation. Through this investigation of the relationship between the structure of the kernel function and the maximisation of the marginal likelihood, the study outlines a clear guideline for choosing an appropriate model by balancing the computation time and model performance through optimal kernel configuration.

1.1 Research Focus and Justification

As earlier stated, rainfall intensity predictions are crucial for managing floods, water systems, agriculture, and hydrotechnical facilities (Ekpenyong et al., 2009; Ibrahim et al, 2022)). Traditional physical models typically demand many parameters and lengthy calibration procedures, making them difficult to implement in areas lacking comprehensive meteorological and topographical data.

In the last few decades, GPR has become increasingly popular in the field of non-parametric machine learning due to its effectiveness when dealing with small-sized data sets while simultaneously avoiding underfitting and overfitting problems.

Compared with other machine learning methods, such as neural networks, GPR is particularly advantageous as a black-box technique since it provides a full distribution as an output in addition to a prediction value, which means the confidence interval can be estimated for assessing hydrological risks. The key issue regarding GPR in data predictive learning is related to its computational complexity as well as kernel choice (Isabona and Ojuh, 2021).

In GPR, there is a problem of cubic scaling. Besides, rainfall data is generally non-stationary and multi-scale. Choosing an unsuitable kernel can cause a problem of poor generalisation. Some kernels can either overly smooth the peaks of rainfall or ignore seasonal periodicities. This research is aimed at addressing and determining the non-linear relationship and high variability of precipitation intensity through GPR-based kernel selection and integration. Via the aim, the following contribution to knowledge has been made:

- Developed an integrated forecasting framework by combining the GPR learning method with the Bayesian optimisation method to improve prognostic approximation accuracy in precipitation data mining.
- Utilized the non-parametric developed integrated GPR method to better model the spatial distribution of non-Gaussian precipitation variables, which often has skewed probability distributions that standard GPR may struggle to capture.
- Compared various single (SE, Matérn, RQ) and combined (sum or product of pairs) kernels to evaluate their ability to capture complex, non-linear systematic prediction errors in hydrological models.
- Generated mean approximation estimates alongside uncertainty estimates to provide essential confidence measures for early warning systems and flood control.

2. Theoretical Framework

A Gaussian Process is defined as a distribution over functions:

$$y = f(x) + \varepsilon \qquad (1)$$

$$f(x) = GP(m(x), k(x, x')). \quad (2)$$

For a dataset with N observations, the training process requires computing the N x N matrix and solving for the marginal log-likelihood, which involves the inverse of k.

This can be achieved by engaging the Bayesian optimisation method to iteratively update the hyper-parameters k(x, x') and covariance kernels to maximise the marginal log-likelihood. The nine kernels under investigation in this paper include the exponential, marten32, matern52, ard-exponential, ard-marten32, ard-matern52, squared-exponential, ard-squared-exponential, and ard-rational-quadratic kernels.

3. Literature Review: Kernels in Hydrological Flux

The primary challenge in GPR is the inversion of the covariance matrix (K) (Isabona and Ojuh, 2021). For N rainfall data training points, the GPR training process involves a complexity computation of $O(N^3)$. In practice, the Squared Exponential kernel is generally used to model rainfall because of its "smoothness" property. However, rainfall is not smooth but highly intermittent and volatile Isabona et al, (2023). According to Rasmussen and Williams (2006), theoretically, even though RBF is infinitely differentiable, it tends to over-smooth hydrological peaks.

Chen et al. (2020) have shown that by using one kernel alone, such as RBF, it cannot represent the seasonal cycle of the 12-month monsoon. Their analysis proved that there was a substantial improvement in R^2 score when the Composite Kernel (RBF+Periodic) is applied. Nonetheless, their findings also revealed that there is an additional training cost of about 45%, as both length-scale and period parameters needed to be optimised together.

Rainfall processes have been considered to operate on different length scales, both convective (small-scale) and synoptic (large-scale)(Ibrahim et al, 2022). In Sun et al. (2019) work, an investigation on the Rational Quadratic (RQ) kernel application, which functions as a scale mixture of RBF kernels, was conducted. Based on their findings, RQ had better predictive performance compared to RBF for monthly precipitation intensities due to its ability to capture changes on multiple scales. However, in computational terms, RQ proved to be more sensitive to initial hyper-parameter settings, sometimes resulting in longer training time due to getting stuck in "local minima traps."

To overcome the problem of cubic complexity $O(N^3)$: The idea of Sparse GPR was brought forward by Titsias (2009), introducing the concept of "inducing points." As regards rainfall, Liu et al. (2022) tested the application of Sparse GPR approach to a 50-year data set on monthly precipitation. They observed that although complex kernels' combination (Matern + Periodic) turned out to be impossible to use in the ordinary GPR setup due to high computational cost, they proved to be feasible using the Sparse GPR approach.

This paper is specifically focused on a thorough comparative training time and computational complexity analysis of the effect of nine different covariance functions on the modelling of monthly rainfall data using the Bayesian optimisation empowered GPR method.

4. Research Methodology for Rainfall Intensity Prediction

To address the research objectives outlined above, we implemented a robust, structured, and stepwise Bayesian optimisation framework designed to fine-tune the hyper-parameters of the Gaussian Process Regression (GPR) model. This process involved a multi-stage optimisation process where the marginal likelihood function is iteratively evaluated to select the most representative kernel parameters (such as length-scale and rainfall intensity amplitude). By structuring the optimisation in this way, we ensured that the GPR model could effectively capture the complex, non-linear variability inherent in monthly rainfall data, leading to more precise and reliable estimations across diverse temporal scales. Given the stochastic nature of rainfall patterns, this approach systematically explored the hyper-parameter space to identify optimal kernel configurations. By iteratively refining these parameters through a Bayesian lens, we aimed to maximise the predictive accuracy of our model in estimating long-term monthly rainfall intensities while simultaneously mitigating the risks of overfitting and computational inefficiency common in high-dimensional meteorological datasets. The breakdown of the process is as follows:

(i) **Data Preprocessing and Partitioning**:

- The Rainfall datasets were split into training (e.g., 80%) and testing (20%) subsets.
- Moving average filters have been used to smooth input data and improve model robustness.

(ii) Kernel Selection and Construction:

- Single kernels (Exponential, Matern32, Matern52) or mixture kernels (combining Squared Exponential, Periodic, and Rational Quadratic terms) were selected to reflect trend, periodicity, and randomness in rainfall.

(ii) **Hyper-parameter Optimisation**:

- Models were trained by maximising the **marginal likelihood** (also called marginal possibility) based on observed data.
- Optimisation typically utilises gradient descent to identify patterns and refine the model's posterior distribution of weights.

(iv) Performance Evaluation:

- The standard metric used in this paper to examine the computation efficiency of the kernel function-based GPR process is the Root Mean Square Error (RMSE), and it measures the mean difference between approximated and actual observed rainfall intensity values, with lower values indicating better computational efficiency and accuracy.
- We also engaged the precision training time of the kernel function-based GPR process to examine the computational cost (complexity) on the observed rainfall intensity data at different volumes as shown in Table 2.

4.1 Matlab Implementation Codes

Here, MATLAB was used to design and implement the focused structured, and systematic GPR-based Bayesian optimization algorithm with numerous kernel function hyperparameters:

```
% Monthly Rainfall Intensity Prediction Comparison comes in Matlab
% Load the rainfall intensity data
load rainfallData.mat
 X=Data(:,1); %Monthly data
 Y=Data(:,2);% rainfall intensity
% 1. Squared Exponential Kernel
tic;
gprSE = fitrgp(X, Y, 'KernelFunction', 'squaredexponential', 'Standardize', true);
timeSE = toc;

% 2. Matern 5/2 Kernel (Less smooth, often better for natural phenomena)
tic;
```

```
gprMatern = fitrgp(X, Y, 'KernelFunction', 'matern52', 'Standardize', true);
timeMatern = toc;

% 3. Combined Custom Kernel (Sum of Squared Exponential and Rational Quadratic)
% Note: Requires defining initial parameters (theta)
kernel1 = @(x1,x2,theta) exp(-theta(1)*(pdist2(x1,x2).^2));
kernel2 = @(x1,x2,theta) (1 + pdist2(x1,x2).^2/(2*theta(2)*theta(3))).^(-theta(3));
combinedKernel = @(x1,x2,theta) (kernel1(x1,x2,theta(1)) + kernel2(x1,x2,theta(2:3)));
initialTheta = [1, 1, 1];
tic;
gprCombined = fitrgp(X, Y, 'KernelFunction', combinedKernel, 'KernelParameters', initialTheta);
timeCombined = toc;

% Prediction and Performance Metrics
[ypred, ysd, yint] = predict(gprMatern, Xtest);
mseValue = loss(gprMatern, Xtest, Ytest);
fprintf('SE Time: %.4f s\nMatern Time: %.4f s\nCombined Time: %.4f s\n', timeSE, timeMatern, timeCombined)
```

5. Results and Discussion

The results in figures 2-4 show that computational complexity of GPR is mainly driven by the number of training observations (N) rather than the specific kernel chosen, typically scaling as $O(N^3)$. However, in term of computation efficiency as revealed in the same figures, the graphs also real that choice of kernel significantly affects training time because more complex kernels require more iteration to optimize additional hyper-parameters or handle less stable numerical operations.

Particularly, the results in figures 1-4 and Tables 1-2, show that the mixture kernels, namely ArdExponential, ArdMatérn32 and ArdMatern52 kernels produced the best computational efficiency and complexity of the GPR learning process. The attained optimal performance can be attributed to their respective ability to match the intermittent behaviour of the precipitation characteristics better than kernels. This result clearly indicates that the mixture of Automatic Relevance Determination (Ard) with the Exponential, Matern32 and matern52 kernels can be used to identify the most significant input features of the observed rainfall intensity data. As far as computational efficiency is concerned, the results show that the ArdMatérn kernels take more time than ArdExponential, but only a little extra in terms of the number of training cycles. However, the improvements in RMSE are remarkable.

Although the Matern32 and Exponential kernels attained relatively good computational efficiency, they failed to perform optimally in terms of training time when observed monthly rainfall data were increased. There is usually a sudden change in the intensity of the rain, for example, a sudden start of the monsoon season or even drought. Since the Exponential kernel is too smooth, it is likely to "oversmooth" thus generating very small intervals which do not cover the sudden changes in the intensity of the rainfall.

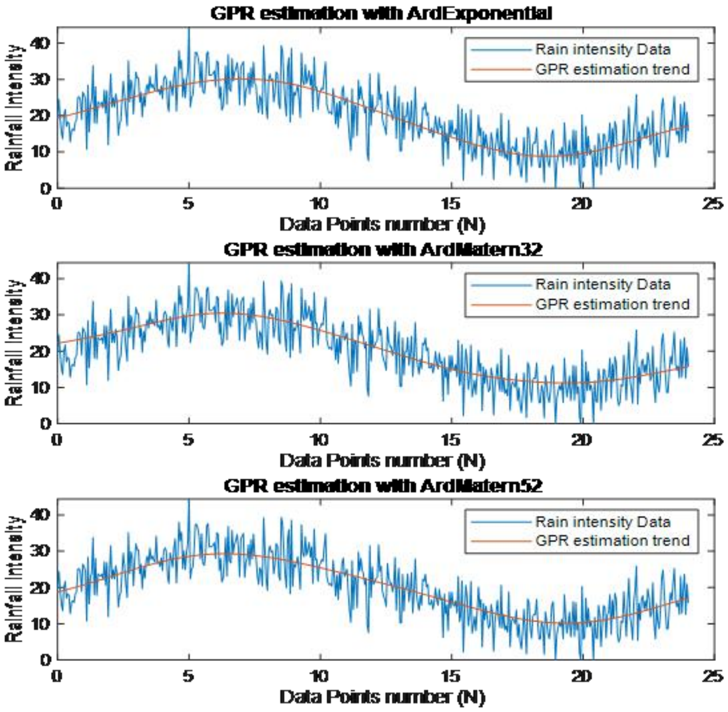

Figure 1: The GPR estimation results of the GPR with ArdExponential, ArdMatern32 and ArdMatern52 kernels

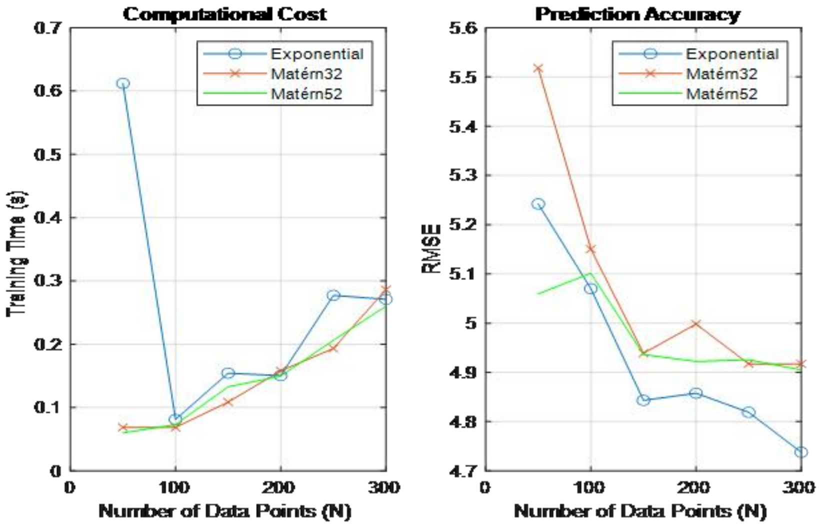

Figure 2: GPR Computational Cost and Computation Efficiency with Exponential, Matern32 and Matern52 kernels on Rainfall intensity data number

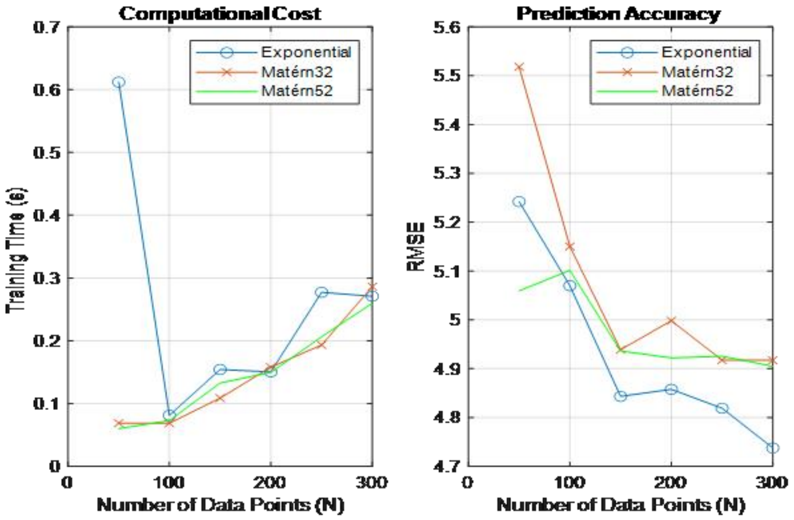

Figure 3: GPR Computational Cost and Computation Efficiency with ArdExponential, ArdMatern32 and ArdMatern52 kernels on Rainfall intensity data number

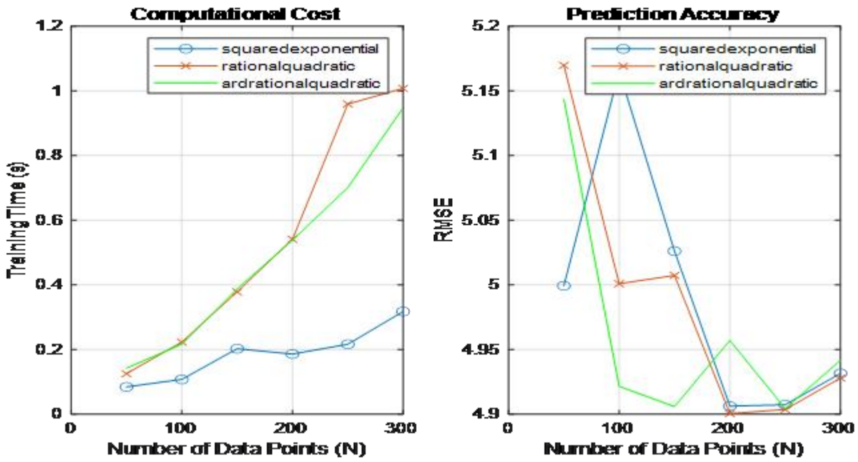

Figure 4: GPR Computational Cost and Computation Efficiency with SquareExponential, Rationalquadratic and ArdRationalquadratic on Rainfall intensity data number

Table 1: GPR Computation Efficiency on different Rainfall intensity data number

	Computational Efficiency (db))					
Kernel Functions	50	100	150	200	250	300
Exponential	5.24	5.07	4.84	4.86	4.82	4.74
Matern32	5.52	5.15	4.94	5.00	4.92	4.92
Matern52	5.06	5.10	4.94	4.92	4.93	4.91
Ardexponential	4.82	4.97	4.73	4.70	4.61	4.60
ArdMatern32	4.83	4.78	4.77	4.78	4.72	4.70
ArdMatern52	4.89	5.03	4.74	4.71	4.72	4.73
Squared Exponential	5.00	5.17	5.03	4.91	4.91	4.93
Rational Quadratic	5.17	5.00	5.01	4.90	4.90	4.93
ArdRationalQuadratic	5.14	4.92	4.91	4.96	4.90	4.94

Table 2: GPR Computation Cost on different Rainfall intensity data number

Kernel Functions	Computational Complexity (s)					
Exponential	50	100	150	200	250	300
Matern32	0.61	0.08	0.15	0.15	0.28	0.27
Matern52	0.07	0.07	0.11	0.16	0.19	0.29
Ardexponential	0.06	0.07	0.13	0.15	0.21	0.26
ArdMatern32	0.09	0.10	0.17	021	0.35	0.36
ArdMatern52	0.10	0.10	0.18	0.21	0.28	0.36
Squared Exponential	0.09	0.11	0.17	0.22	0.31	0.41
Rational Quadratic	0.08	0.11	0.20	0.19	0.22	0.32
ArdRationalQuadratic	0.12	0.22	0.38	0.54	0.96	1.10
Different Rain Intensity	0.14	0.22	0.39	0.54	0.70	0.95

6. Conclusion

Rainfall intensity is characterized by high non-linearity, seasonality, and stochastic noise. GPR is favoured in this domain for its ability to provide uncertainty quantification alongside point estimates. The core of a GPR model is the kernel function k(x, x'), which defines the covariance between data points. While model performance is often the primary metric, the computational burden, specifically matrix inversion makes kernel selection a critical performance decision in large-scale meteorological datasets.

The Computational Complexity and Training Time Synthesis of Gaussian Process Regression Kernels for Monthly Rainfall Intensity Estimation conducted in this paper reveals that the mixture kernels, namely ArdExponential, ArdMatérn32 and ArdMatern52 kernels produced the best computaional effienciency and complexity of the GPR learning process. While the Matern and Rational Quadratic kernels offer the most "accurate" representation of the attenuating nature of precipitation, they demand robust optimization strategies. The results of the selected GPR kernels for the monthly rainfall intensity estimation show a balancing act between physical realism and computational feasibility. Future research appears to be moving away from finding the "perfect kernel" and toward Hybrid GPR architectures, where sparse approximations allow for the use of highly complex, multi-layered kernels that were once computationally impossible.

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