Surface Reconstruction of 3D Point Clouds Using Linear and Gaussian Process Regression: Model Evaluation and Hyperparameter Optimization

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***Abstract*—This project explores surface modeling techniques applied to 3D point cloud data of buildings and terrain, focusing specifically on Linear Regression (LR) and Gaussian Process Regression (GPR). For modeling wall surfaces, LR was utilized with automatic dimensionality selection based on the lowest mean squared error (MSE). In contrast, GPR was employed to estimate complex terrain surfaces, providing both accurate predictions and quantified uncertainty estimations. Furthermore, we systematically evaluated both models and addressed the challenges associated with manual hyperparameter tuning by implementing Maximum Likelihood Estimation (MLE), significantly improving the predictive performance of GPR. Our results demonstrate the effectiveness of automated parameter optimization and rigorous model evaluation, highlighting their potential in robotic navigation, environmental modeling, and adaptive learning scenarios.**

I. Introduction

Accurate surface modeling from 3D point cloud data plays a critical role in robotic perception, supporting essential tasks such as autonomous navigation, manipulation, environmental understanding, and obstacle avoidance [1], [2]. Among various techniques, regression methods have gained popularity for surface reconstruction due to their efficiency and interpretability. Linear regression, in particular, stands out for its simplicity and computational speed, making it well-suited for initial approximations or modeling planar structures [3]. However, the performance of linear models often decreases significantly in real-world scenarios, which usually involve complex nonlinearities, noise, and uncertainties.

Gaussian Process Regression (GPR) effectively addresses these challenges by providing a flexible, probabilistic framework capable of modeling complex nonlinear relationships while simultaneously quantifying uncertainties [4], [5], [6]. The ability to estimate uncertainties is particularly valuable in robotics, as it allows robots to make safer and more informed decisions under uncertain conditions [2]. Nevertheless, the effectiveness of GPR is highly dependent on appropriate kernel hyperparameters, which traditionally require significant manual tuning, making the modeling process inefficient and less practical.

In this assignment, we systematically explore both linear and Gaussian process regression methods by applying them to surface modeling of walls and terrains extracted from real-world point cloud datasets. To objectively evaluate these methods, we employ metrics such as Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and uncertainty analysis [7]. Additionally, we implement an automated hyperparameter optimization approach using Maximum Likelihood Estimation (MLE) [8], [9], thereby significantly reducing manual tuning efforts and improving model performance.

The main contributions of this assignment are as follows:

- Implementation and systematic evaluation of linear regression and Gaussian Process Regression for robotic surface modeling tasks.
- Development of an automatic hyperparameter optimization method for Gaussian Process models to avoid manual tuning.
- A comprehensive strategy for analysis and visualization that integrates predictive accuracy with uncertainty estimation.

The structure of this report is organized as follows: Section 2 introduces the methodologies and model implementations. Section 3 presents experimental results and performance evaluations. Section 4 discusses and analyzes the findings, and Section 5 summarizes the contributions of this assignment and briefly outlines directions for future work.

II. Methodology

A. Linear Regression

This section outlines the methodology adopted to perform surface reconstruction using linear regression. The approach consists of two main steps: preprocessing the raw point cloud data and fitting a linear model to approximate surfaces within clusters.

1) Dataset and Preprocessing: The original dataset consists of three-dimensional point clouds captured from a real-world environment. To facilitate effective surface modeling, the point clouds corresponding to building structures were isolated using DBSCAN clustering. Each identified cluster represents a coherent surface or plane, suitable for linear approximation.

After clustering, we employed a grid-based regularisation technique termed *bounding grid*, to uniformly sample points from the irregularly distributed cloud data. The bounding grid method constructs an evenly spaced set of points within the spatial bounds of each cluster, significantly improving computational efficiency and visualization clarity.

Formally, given n original data points $\{\mathbf{x}_i\}_{i=1}^n$, where $\mathbf{x}_i \in \mathbb{R}^3$, the regularized grid points $\mathbf{x}_{\text{grid}}$ are defined by:

$$\mathbf{x}_{\text{grid}} = \text{bounding\_grid}\left(\{\mathbf{x}_i\}_{i=1}^n\right)$$

This process replaces the irregular point set with a structured grid having approximately the same number of points, providing uniform coverage and enhanced visualization of the cluster's geometric structure.

2) Linear Model Fitting: The primary objective of linear regression in this context is to identify and approximate planar surfaces within each cluster. Given that each point is defined by three coordinates (x, y, z), we formulate three potential regression problems, each using two coordinates as input features and the remaining one as the target variable. Specifically, for each cluster, we test the following linear models:

$$\begin{aligned} z &= \beta_{0,z} + \beta_{1,z}x + \beta_{2,z}y \\ y &= \beta_{0,y} + \beta_{1,y}x + \beta_{2,y}z \\ x &= \beta_{0,x} + \beta_{1,x}y + \beta_{2,x}z \end{aligned}$$

Here, β parameters are estimated using the Ordinary Least Squares (OLS) method, which minimizes the Mean Squared Error (MSE):

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

The regression direction (i.e., the choice of the dependent variable among x, y, or z) that yields the lowest MSE is selected as the best linear approximation of the corresponding cluster.

Subsequently, the chosen linear model is used to predict the values on the structured grid points generated previously. The predicted coordinates, combined with the regularized grid, produce a linearly approximated surface representation of each cluster.

3) Model Evaluation and Visualization: The effectiveness of linear regression approximation is evaluated quantitatively and qualitatively. Quantitative assessment involves computing per-cluster MSE and the coefficient of determination R^2, defined as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

where y_i are true values, $\hat{y}_i$ are predictions, and $\bar{y}$ is the mean of observed values. Higher R^2 indicates a better fitting performance.

Qualitative assessment is achieved through visualization. Figures 1 and 2 depict the original clustered point cloud and the corresponding fitted surfaces, respectively. Additionally, Figures 3 and 4 illustrate the per-cluster evaluation metrics.

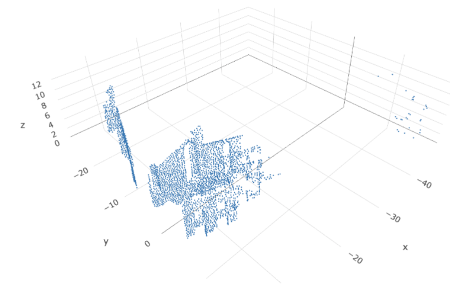

Fig. 1. Original clustered building point cloud before linear approximation.

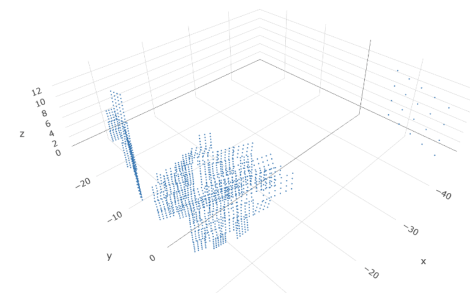

Fig. 2. Linear regression approximated surface for each cluster using bounding-grid regularisation.

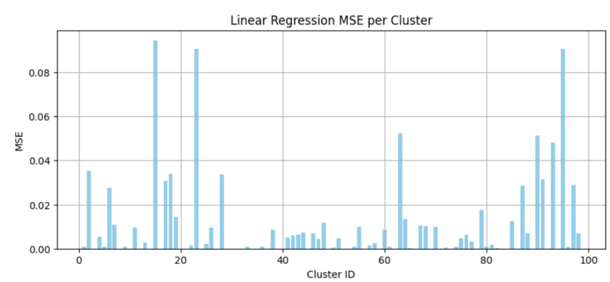

Fig. 3. Mean Squared Error (MSE) of linear regression per cluster. Lower MSE indicates better surface fitting.

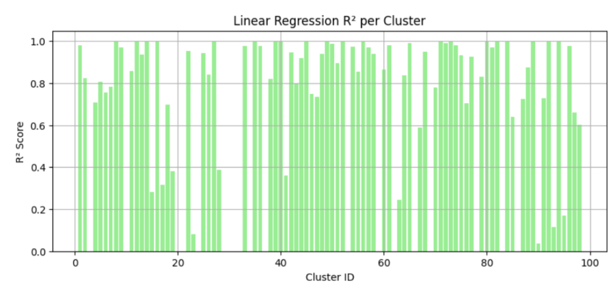

Fig. 4. Coefficient of determination (R^2) per cluster, indicating how well the linear regression fits the data. Values closer to 1 denote better fits.

This structured approach clearly illustrates the efficiency and limitations of linear regression for surface approximation tasks in robotics contexts, guiding us towards the more sophisticated Gaussian Process Regression presented in the subsequent section.

B. Gaussian Process Regression

1) Overview: Gaussian Process Regression (GPR) is a non-parametric, probabilistic approach to regression that is particularly effective in modeling nonlinear surfaces. Unlike linear models, GPR assumes a distribution over functions and produces not only the predicted mean but also a measure of uncertainty for each prediction [4], [5]. This is especially beneficial in robotic applications, where uncertainty estimation plays a critical role in safe planning and decision-making [1].

The GPR model assumes that the function $f(\mathbf{x})$ follows a Gaussian Process:

$$f(\mathbf{x}) \sim \mathcal{GP}(0, k(\mathbf{x}, \mathbf{x}'))$$

where the kernel function $k(\cdot, \cdot)$ determines the smoothness and generalization ability of the model. In our case, we use the squared exponential kernel:

$$k(\mathbf{x}, \mathbf{x}') = \sigma_f^2 \exp\left(-\frac{\|\mathbf{x} - \mathbf{x}'\|^2}{2\ell^2}\right)$$

where ℓ is the lengthscale and σ_f^2 is the signal variance.

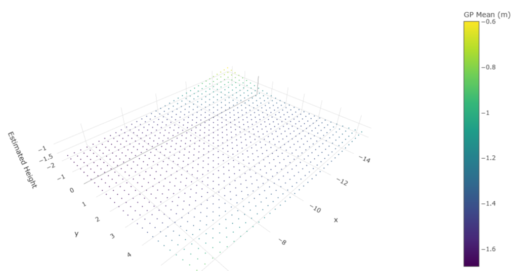

Fig. 5. Gaussian Process estimated surface (mean predictions)

2) Prediction Formulation: Given training inputs $\mathbf{X}_d \in \mathbb{R}^{n \times 2}$ and targets $\mathbf{y}_d \in \mathbb{R}^n$, the posterior predictive distribution at query points $\mathbf{X}_q$ is given by:

$$\boldsymbol{\mu}_q = K_{qd}(K_{dd} + \sigma_n^2 I)^{-1} \mathbf{y}_d$$

$$\Sigma_q = K_{qq} - K_{qd}(K_{dd} + \sigma_n^2 I)^{-1} K_{dq}$$

where:

- $K_{dd} = k(\mathbf{X}_d, \mathbf{X}_d)$
- $K_{qd} = k(\mathbf{X}_q, \mathbf{X}_d)$
- $K_{dq} = K_{qd}^\top$, $K_{qq} = k(\mathbf{X}_q, \mathbf{X}_q)$
- σ_n is the assumed observation noise

The predictive standard deviation is obtained from:

$$\sigma_q = \sqrt{\operatorname{diag}(\Sigma_q)}$$

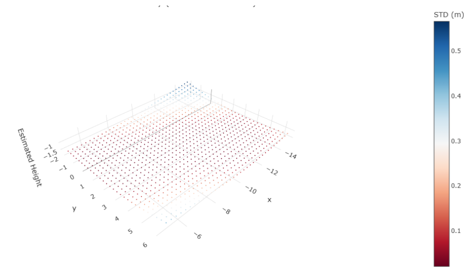

Fig. 6. Predicted standard deviation (uncertainty) using GPR

3) Hyperparameter Optimization with MLE: The performance of GPR is highly dependent on the kernel hyperparameters ℓ and σ_f. Rather than manually tuning them, we use Maximum Likelihood Estimation (MLE) to learn optimal values. This is done by minimizing the negative log marginal likelihood:

$$\mathcal{L}(\ell, \sigma_f) = \frac{1}{2}\mathbf{y}_d^\top (K_{dd}+\sigma_n^2 I)^{-1}\mathbf{y}_d + \frac{1}{2}\log|K_{dd}+\sigma_n^2 I| + \frac{n}{2}\log 2\pi$$

We search over multiple initializations using L-BFGS-B optimization to avoid local minima. This step significantly improves the model without manual parameter selection.

4) Interactive Visualization: We also implemented an interactive 3-in-1 plot for visualizing ground truth, predicted surface, and uncertainty. This tool aids interpretation and debugging during development.

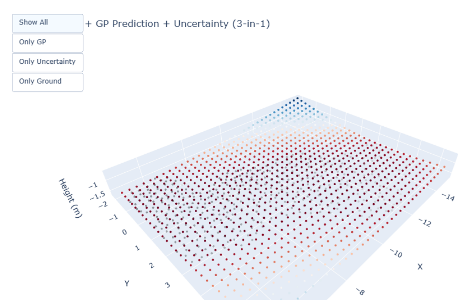

Fig. 7. Interactive view combining ground truth, GP prediction, and uncertainty

5) Quantitative Evaluation: We quantitatively evaluate the GPR model using Mean Squared Error (MSE), Root Mean Squared Error (RMSE), and average predictive uncertainty:

$$\text{MSE} = \frac{1}{n}\sum_i (\hat{y}_i - y_i)^2 \quad , \quad \text{RMSE} = \sqrt{\text{MSE}} \quad , \quad \bar{\sigma} = \frac{1}{n}\sum_i \sigma_i$$

- MSE = 0.1053
- RMSE = 0.3245
- Mean predicted standard deviation = 0.1534

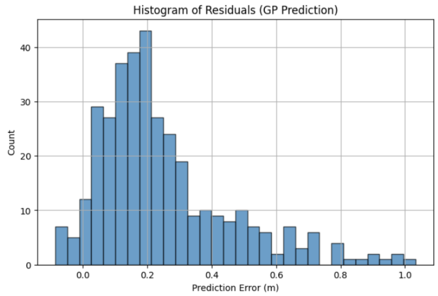

Fig. 8. Histogram of residuals showing prediction error distribution

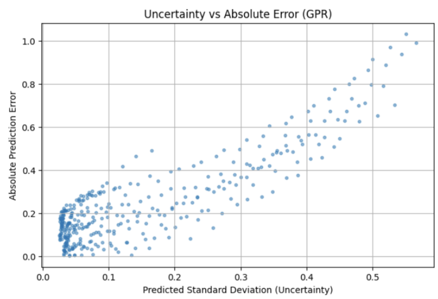

Fig. 9. Scatter plot: predicted uncertainty vs actual prediction error

III. Discussion and Conclusion

This section presents a comparative discussion of the results obtained from the linear and Gaussian process regression (GPR) models. The analysis focuses on prediction accuracy, generalization capacity, and the ability to estimate uncertainty.

A. *Performance of Linear Regression*

Linear regression was applied independently to each wall cluster. For every cluster, we selected the best regression direction (x, y, or z) based on the minimum Mean Squared Error (MSE). While the model is computationally efficient and performed well on near-planar surfaces, its simplicity limits its expressiveness in more complex geometric settings.

Figure 1 and Figure 2 compare the raw and fitted results, showing good alignment in flat regions. However, the evaluation metrics in Figure 3 and Figure 4 indicate performance degradation for certain clusters, especially those with curvature or noise. This reveals the limitation of using a global linear model in local, irregular structures.

B. *Performance of Gaussian Process Regression*

In contrast, GPR provides a probabilistic and flexible framework for modeling continuous surfaces with spatially varying smoothness. It not only fits the data well, but also quantifies prediction uncertainty, which is critical in real-world robotic scenarios.

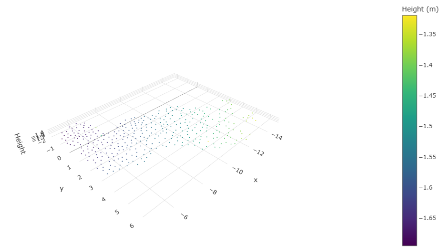

Fig. 10. Original segmented wall point cloud

The GP results are shown in Figures 10, 5, and 6, demonstrating accurate modeling and smooth transitions across the terrain. Using Maximum Likelihood Estimation (MLE) for kernel hyperparameters significantly improved the quality of prediction while eliminating the need for manual tuning.

Figure 7 further integrates the ground truth, GP prediction, and uncertainty into a single 3D view for intuitive analysis.

C. *Quantitative Evaluation*

The evaluation metrics summarize the contrast between the two methods:

- **Linear Regression:** Effective on planar surfaces but suffers on curved or noisy regions.
- **GPR:** Achieved MSE of 0.1053, RMSE of 0.3245, and a mean predicted standard deviation of 0.1534.

The residual histogram in Figure 8 shows that most GPR errors are centered near zero. Furthermore, Figure 9 confirms a strong correlation between predicted uncertainty and actual error, validating the reliability of uncertainty estimation.

D. *Conclusion*

This assignment systematically investigated two regression models for 3D surface modeling from point cloud data. Linear regression proved to be fast and effective for simple structures but lacked generalization capacity. GPR, empowered by MLE-based optimization, demonstrated superior accuracy and uncertainty-aware modeling, making it a better choice for applications in autonomous robotics and terrain analysis.

In summary, the results highlight the importance of combining predictive accuracy and uncertainty estimation in real-world robotics. Future work may explore online GPR, sparse approximations for large datasets, and applications to dynamic or partially observed environments.

IV. Reflection

This assignment was completed smoothly in terms of basic implementation. Both linear regression and Gaussian Process Regression (GPR) were successfully applied to real-world point cloud data to reconstruct surfaces. However, I did not stop at completing the core requirements; instead, I proactively explored deeper model evaluation and optimization.

After initial implementation, I noticed that the Gaussian Process model exhibited suboptimal performance. I began manually tuning the kernel hyperparameters—namely the `lengthscale` and signal variance σ_f—to understand their influence on prediction accuracy and uncertainty calibration. Through this process, I discovered a crucial trade-off between low error and proper uncertainty estimation. For example, the model with `lengthscale` = 5.0 and $\sigma_f = 0.7244$ yielded the lowest MSE (0.0332), but its predicted uncertainty (mean STD = 0.0777) was far lower than the actual RMSE (0.1822), indicating overconfidence. In contrast, a more balanced configuration with `lengthscale` = 3.0 and $\sigma_f = 0.6792$ produced slightly higher MSE (0.1053), but with a more realistic uncertainty level (mean STD = 0.1534).

Realizing the complexity of manual tuning, I further explored and implemented a Maximum Likelihood Estimation (MLE) framework to automate kernel parameter optimization. This not only improved predictive performance but also ensured that the uncertainty estimates were better aligned with actual prediction error. The process of integrating MLE into the GPR pipeline significantly enhanced the model's robustness and reduced human effort.

Overall, this reflection highlights the importance of moving beyond standard evaluation metrics such as MSE and RMSE. A well-calibrated model that accurately reflects its confidence is essential in robotics and real-world decision-making. In the future, I plan to explore post-hoc uncertainty calibration techniques and alternative probabilistic models to further improve model trustworthiness.

References

[1] M. Arduengo, A. Colomé, J. Lobo-Prat, L. Sentis, and C. Torras, "Gaussian-process-based robot learning from demonstration," *Journal of Ambient Intelligence and Humanized Computing*, 2023. [Online]. Available: https://link.springer.com/article/10.1007/s12652-023-04551-7

[2] D. Forte, A. Ude, and A. Kos, "Robot learning by gaussian process regression," in *2008 7th IEEE International Conference on Development and Learning*. IEEE, 2008, pp. 272–277. [Online]. Available: https://www.researchgate.net/publication/224160958_Robot_learning_by_Gaussian_process_regression

[3] R. Falque, "Ai in robotics: Supervised learning – linear regression (week 04)," 2024, lecture Slides, UTS Robotics Institute.

[4] C. E. Rasmussen and C. K. I. Williams, *Gaussian Processes for Machine Learning*. MIT Press, 2006. [Online]. Available: https://gaussianprocess.org/gpml/

[5] L. Wu, "Ai in robotics: Non-linear regression with gaussian process (week 05)," 2024, lecture Slides, UTS Robotics Institute.

[6] C. K. I. Williams, "Prediction with gaussian processes: From linear regression to linear prediction and beyond," *NATO ASI Series F: Computer and Systems Sciences*, vol. 168, pp. 599–621, 1998.

[7] D. Chicco and G. Jurman, "The coefficient of determination r² is more informative than smape, mae, mape, mse and rmse in regression analysis evaluation," *PeerJ Computer Science*, vol. 7, p. e623, 2021.

[8] K. P. Murphy, *Machine Learning: A Probabilistic Perspective*. MIT Press, 2012.

[9] J. Shawe-Taylor and N. Cristianini, *Kernel Methods for Pattern Analysis*. Cambridge University Press, 2004.