Introduction to Gaussian Processes

Presenter: Yan Peng
Mentor: Yuhan Qian

Gaussian Processes (GPs) are a foundational tool in machine learning, particularly for problems involving regression and uncertainty quantification. This presentation outlines the evolution of modeling from linear regression to GPs, emphasizing their benefits in capturing complex relationships and offering robust predictive capabilities.

Linear Regression

Linear regression is a simple yet computationally efficient model with clear interpretability. However, it struggles to capture non-linear patterns and lacks uncertainty quantification. Regularization methods like Ridge Regression address overfitting and improve generalization but introduce bias and may reduce training accuracy.

Bayesian Regression

Moving beyond deterministic approaches, Bayesian regression incorporates prior distributions and updates them with observed data, enabling probabilistic predictions. This framework lays the foundation for Gaussian Processes by integrating kernel methods.

Gaussian Processes

A Gaussian Process is a collection of random variables, any finite number of which are jointly Gaussian, defined by a mean function and a kernel (covariance) function. The RBF (Radial Basis Function) kernel is commonly used for its ability to capture smoothness and local variations in the data.

Kernel Ridge Regression (KRR) and GPs

Kernel Ridge Regression provides a bridge to GPs, where the predictive function leverages kernel-defined similarity measures. Key parameters include:

- **Length scale (ρ)**: Determines the smoothness of the model.
- **Regularization (λ)**: Balances bias and variance.

Conclusion

Gaussian Processes offer a powerful, flexible approach to regression, effectively capturing uncertainty and complex patterns. The insights from KRR provide an intuitive foundation, illustrating how parameter tuning affects model behavior.