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Machine Learning Framework for Double Generalized Additive Model

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Abstract

This research develops an enhanced framework for predictive modeling by extending the theoretical foundations of Generalized Additive Models (GAMs). GAMs provide a flexible and interpretable approach for modeling complex nonlinear relationships between a response variable and its predictors through additive smooth functions. However, conventional GAMs primarily focus on modeling the conditional mean and commonly assume constant dispersion and shape parameters. To address these limitations, this research introduces the Double Generalized Additive Model (DGAM), in which additive predictors are specified for both the mean and dispersion components. This dual structure enables explicit modeling of heteroscedasticity and varying uncertainty across observations, which are common in empirical data but inadequately handled by standard GAMs. In addition, the classical spline-based smoothing framework is extended to modern machine learning contexts using Random Forest (RF) and Histogram-based Gradient Boosting Regression Tree. The proposed framework is validated using the health-related dataset from the National Health Insurance Service Health Checkup Database (Korea). Results indicate that models employing a RF–based mean structure achieve the strongest predictive performance among all considered approaches. However, due to the limited heteroscedasticity present in the data, DGAM does not provide additional benefits over the conventional GAM. In contrast, when heteroscedasticity is present, DGAM offers substantially greater flexibility in capturing nonlinear effects in both the mean and dispersion components than the conventional approaches discussed earlier.

Keywords: Generalized Additive Model (GAM); Double Generalized Additive Model (DGAM); Predictive Modeling

Introduction

Mathematical modeling has undergone substantial development over time, evolving from simple linear models and multiple linear regression to response transformation techniques, classical linear models, generalized linear models (GLMs), double generalized linear models (DGLMs), and Generalized Additive Models (GAMs). GAMs can effectively handle nonlinear relationships commonly observed in real-world data (Hastie & Tibshirani, 1986). In predictive modeling, the fundamental task is to characterize the relationship between explanatory variables and a response variable. GAMs employ smoothing functions, such as spline-based smoothers or nonparametric regression techniques, to allow the estimated relationship to adapt to the underlying structure of the data. However, conventional GAMs primarily focus on modeling the conditional mean while requiring the dispersion parameter to be specified or assumed a priori. If the dispersion is improperly specified, the resulting mean function may become distorted, thereby undermining the reliability and interpretability of the inferred nonlinear relationships. To address this limitation, this research proposes modeling both the mean and dispersion components within an additive framework, leading to the Double Generalized Additive Model (DGAM). Furthermore, to enhance the efficiency and expressive power of the smoothing process, modern machine learning techniques, including tree-based

ensemble methods and deep distributional neural networks, are incorporated to construct flexible and data-adaptive smoothing functions.

Methodology / Proposed Approach

This work proposes a theoretical concept of DGAM by assuming two additive predictors and link functions follow the exponential family assumption. The modeling step starts by fixing the dispersion value, then finding the fitting curve for the mean, calculate the suitable curve for the dispersion, and repeat the steps until the acceptable error. For parameter estimation, classical spline-based techniques and two machine learning approaches are employed: Histogram-based Gradient Boosting Regression Tree (GBR), and Random Forest (RF). Consequently, a total of three GAMs and nine DGAMs are constructed, accounting for all combinations of estimation methods applied to both the mean and dispersion components. The proposed models are applied to large-scale health-related data obtained from the National Health Insurance Service Health Checkup Database (Korea), which includes information on height, weight, waist circumference, blood pressure, blood glucose levels, blood lipid profiles, hemoglobin concentration, serum creatinine, and liver enzyme levels (SGOT, SGPT, and GGT). The original dataset consists of 1,000,000 records; after removing incomplete observations, 286,996 records remain for analysis. In this study, 14 health-related variables are used as predictors to estimate serum creatinine and gamma-glutamyl transferase (GGT). Model performance is evaluated using Mean Absolute Error (MAE), Root Mean Squared Error (RMSE), the coefficient of determination (R^2), Continuous Ranked Probability Score (CRPS), Prediction Interval Coverage Probability (PICP), and Gaussian Negative Log-Likelihood (NLL).

Experimental Results & Discussion

The results indicate that, for both serum creatinine and GGT prediction, models employing a random forest (RF) for the mean component achieve the best point prediction performance, as reflected by the lowest RMSE and MAE values and the highest R^2. Specifically, for serum creatinine, the RF-based model yields RMSE = 0.26367, MAE = 0.12456, and R^2 = 0.26754, while for GGT the corresponding values are RMSE = 37.35769, MAE = 15.47512, and R^2 = 0.45492. These findings suggest that the RF approach is more effective in capturing the underlying mean structure than alternative methods. However, DGAM does not demonstrate superior performance when evaluated using probabilistic and uncertainty-related metrics, including NLL, CRPS, and PICP. Overall, the best-performing models are the GAMs with RF-based mean components. In particular, for the serum creatinine model, the GAM achieves NLL = 0.08587, CRPS = 0.10351, and PICP = 0.98652, while for the GGT model, the corresponding values are NLL = 5.03948, CRPS = 14.95697, and PICP = 0.97135.

Conclusion

The experimental results indicate that models with a random forest–based mean structure achieve the best overall predictive performance. However, due to the limited heteroscedasticity present in the data, DGAM does not provide additional benefits over the conventional GAM. For datasets exhibiting heteroscedasticity, DGAM can provide enhanced flexibility for modeling nonlinear effects in both the mean and dispersion relative to conventional methods.

References

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