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what is GAMI-Tree

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The GAMI-Tree is an algorithm developed to fit low-order functional ANOVA (fANOVA) models which are inherently interpretable within the framework of machine learning. This algorithm, a variant of the Generalized Additive Models with Interactions (GAMI), employs model-based trees as base learners and includes a new interaction filtering method that improves the capture of underlying interactions. It also features an iterative training method that converges to a model with better predictive performance and incorporates a "purification" step to ensure interactions are hierarchically orthogonal to main effects. The GAMI-Tree algorithm does not require extensive tuning and is designed to be fast and efficient. It is compared favorably in terms of performance and interpretability to other methods like Explainable Boosting Machines (EBM) and GAMI-Net in scenarios using both simulated and real datasets​​.

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explain how it works

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The GAMI-Tree algorithm is designed to fit models that are interpretable by default, incorporating interaction effects in a structured and clear manner. Here’s a breakdown of how it works:

1. **Base Learning with Model-Based Trees**: The algorithm uses model-based trees as its base learners. Unlike traditional decision trees that primarily focus on partitioning data into homogeneous groups, model-based trees use a model-fitting criterion at each split, aiming to enhance the fit of a specific model at each node. This approach allows for more nuanced captures of interactions between variables.
2. **Interaction Filtering**: One of the key features of GAMI-Tree is its novel interaction filtering method. This method is pivotal for identifying and capturing significant interactions between variables. After the initial fit of the model to the data, the algorithm examines the residuals (the differences between observed and predicted values) to identify where interactions might be improving model performance. It selects these interactions based on their ability to reduce prediction error, rather than just their statistical significance.
3. **Iterative Training Method**: GAMI-Tree uses an iterative training approach that converges to a model with better predictive performance over time. In each iteration, the model updates itself to better capture the underlying structure of the data, refining both the main effects and the interaction terms iteratively. This is different from some other methods that may fit all parts of the model simultaneously, potentially leading to less optimal convergence behaviors.
4. **Purification Process**: To ensure that the model remains interpretable, GAMI-Tree incorporates a purification step. This step makes sure that the interactions are hierarchically orthogonal to the main effects. Hierarchical orthogonality means that the interaction effects do not redundantly encode information that could be explained by main effects alone. This purification is crucial for ensuring that the contributions of interactions to the model are clear and distinct.
5. **Efficiency and Tuning**: The algorithm is designed to be computationally efficient, requiring less extensive hyperparameter tuning compared to other complex models. This makes it more accessible for practical use and faster to deploy on large datasets.

Overall, GAMI-Tree aims to combine the interpretability of generalized additive models with the power of machine learning to capture complex interactions, all while ensuring the model remains understandable and practically useful.

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how is it deifferent from EBM

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GAMI-Tree and Explainable Boosting Machines (EBM) share similar goals in enhancing model interpretability while integrating interactions, but there are key differences in their approach and implementation:

1. **Base Learners**:
   * **EBM** utilizes gradient boosting with piecewise constant trees to fit Generalized Additive Models with Interactions (GAMI). This approach incrementally improves the model by adding trees that address the largest errors of the current ensemble.
   * **GAMI-Tree**, on the other hand, employs model-based trees as its base learners. Model-based trees focus more on fitting a model within each tree node, which can better capture complex patterns and interactions compared to the simpler piecewise constant trees used in EBM.
2. **Interaction Handling**:
   * **EBM** fits interactions using a two-stage approach: first, the main effects are modeled, and then the interactions are added sequentially. This process can sometimes miss or inadequately model interactions that are complex or highly contextual within the data.
   * **GAMI-Tree** incorporates a new interaction filtering method that is better at detecting and modeling underlying interactions. This method is designed to be more effective in capturing significant interactions that directly influence the predictive performance.
3. **Iterative Training and Convergence**:
   * **EBM** follows a typical boosting procedure where trees are added one at a time to reduce residual error, which can lead to a long training process especially as the model complexity increases.
   * **GAMI-Tree** uses an iterative training method that converges more directly to a model with better predictive performance. The iterative refinement of both main effects and interactions helps ensure that each component of the model is optimally adjusted for the overall best performance.
4. **Purification of Interactions**:
   * **EBM** does not explicitly include a step for ensuring that the interactions are hierarchically orthogonal to the main effects. This can sometimes lead to interpretations where the effects of interactions are conflated with main effects.
   * **GAMI-Tree** includes a "purification" step that ensures interactions are hierarchically orthogonal to main effects. This purification process guarantees that the interactions captured by the model do not redundantly include information that can be attributed to main effects, thus enhancing the interpretability of the model.
5. **Implementation Efficiency**:
   * **EBM** can require extensive hyperparameter tuning and may be computationally intensive, especially as the model complexity grows with the inclusion of more interactions.
   * **GAMI-Tree** is designed to be fast and efficient with less need for extensive tuning, making it potentially more suitable for larger datasets or scenarios where model training speed is a priority.

In summary, while both GAMI-Tree and EBM aim to provide interpretable models by integrating interactions, GAMI-Tree introduces advancements in base learning, interaction detection, and model refinement that differentiate it from EBM, particularly in terms of efficiency and the clarity of the interactions modeled.

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The GAMI-Tree algorithm, a robust method for fitting inherently interpretable machine learning models, integrates the principles of Generalized Additive Models (GAMs) with interaction terms to facilitate clearer understanding and usability in predictive modeling. This technical explanation will detail the working of the GAMI-Tree algorithm, highlighting its unique aspects in the context of machine learning interpretability.

**Base Learning Using Model-Based Trees**

The GAMI-Tree algorithm leverages model-based trees as its foundational learners. Unlike traditional decision trees that use simple criteria like Gini impurity or entropy for node splits, model-based trees incorporate a statistical or machine learning model at each node, optimizing a specific model-fitting criterion that can vary depending on the complexity of the data and the interaction structures present (Lou et al., 2013). This allows GAMI-Tree to capture more nuanced interactions between variables efficiently.

**Interaction Detection and Filtering**

One of the standout features of the GAMI-Tree is its interaction filtering method. After fitting an initial model, the algorithm assesses the residuals to pinpoint areas where the model performance can be enhanced through interactions. The selection of these interactions is based on their potential to reduce prediction error significantly, rather than merely on statistical significance, leading to a more practical and performance-oriented model (Hu et al., 2022).

**Iterative Training and Model Refinement**

GAMI-Tree employs an iterative training approach, which refines the model by consecutively updating the main effects and interactions. This method ensures that each component of the model—both main effects and interactions—is optimally adjusted, contributing to an overall better predictive performance. The iterative nature of this training helps in converging more rapidly to a high-performing model compared to traditional methods that might fit all model components simultaneously (Friedman and Popescu, 2008).

**Purification of Interactions**

To ensure that the model remains interpretable and that the interaction terms do not overlap with the main effects, GAMI-Tree includes a purification step. This step ensures that interactions are hierarchically orthogonal to the main effects, meaning that the interaction effects account for variance in the response variable that is not already explained by the main effects alone (Hu et al., 2022). This hierarchical orthogonality is crucial for the clear interpretation of the model, ensuring that the individual contributions of interactions and main effects are well-defined and distinct.

**Computational Efficiency and Implementation**

Designed with practical application in mind, the GAMI-Tree algorithm is implemented to be computationally efficient and requires less intensive hyperparameter tuning than other complex models like deep neural networks or large ensemble models. This efficiency makes GAMI-Tree particularly attractive for large datasets and real-world applications where model training speed and simplicity in tuning are critical (Breiman, 1996).

**Conclusion**

The GAMI-Tree algorithm represents a significant step forward in the development of interpretable machine learning models. By combining the robustness of GAMs with the flexibility and depth of tree-based models, GAMI-Tree offers a powerful tool for both predictive performance and model interpretability. Its unique method of handling interactions, iterative refinement, and efficiency in implementation position it as a preferable choice in scenarios demanding quick, clear, and effective decision-making support.

**References**

* Breiman, L. (1996). Bagging predictors. Machine Learning, 24(2), 123-140.
* Friedman, J. H., & Popescu, B. E. (2008). Predictive learning via rule ensembles. Annals of Applied Statistics, 2(3), 916-954.
* Hu, L., Chen, J., Nair, V. N., & Mukherjee, A. (2022). Using Model-Based Trees with Boosting to Fit Low-Order Functional ANOVA Models. [Journal Name, Volume, Pages].
* Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013). Accurate intelligible models with pairwise interactions. Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining.

These citations offer a glimpse into the theoretical and practical development of the GAMI-Tree algorithm, providing a comprehensive understanding of its operational framework and advantages in the field of interpretable machine learning.

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The GAMI-Tree algorithm stands for Generalized Additive Models with Interactions using Trees. It represents an advanced approach in the realm of interpretable machine learning, providing a robust framework for integrating main effects and interaction terms using boosted model-based trees. Below is a technical explanation of the GAMI-Tree algorithm, incorporating the methodological details, mathematical formulations, and references to key journal articles.

**Mathematical Formulation**

The foundation of the GAMI-Tree algorithm lies in the generalized additive model (GAM) framework, enhanced by incorporating interaction effects. The model can be described as follows:

�(�)=∑�=1���(��)+∑�<����(��,��)*f*(*x*)=∑*j*=1*p*​*gj*​(*xj*​)+∑*j*<*k*​*gjk*​(*xj*​,*xk*​)

Here:

* �(�)*f*(*x*) represents the overall model prediction.
* ��(��)*gj*​(*xj*​) are the smooth functions representing the main effects of each predictor ��*xj*​.
* ���(��,��)*gjk*​(*xj*​,*xk*​) are the interaction terms between predictors ��*xj*​ and ��*xk*​.

**Base Learning Using Model-Based Trees**

GAMI-Tree utilizes model-based decision trees as its base learners. These trees are not just simple partitions of the data but fit a specific model at each node, optimizing a given criterion that relates directly to the GAM structure:

�=�0+�1�1+⋯+����+�*Y*=*β*0​+*β*1​*X*1​+⋯+*βp*​*Xp*​+*ϵ*

Each tree in the ensemble focuses on improving the fit by reducing the residual variance left by previous trees, thereby enhancing both accuracy and interpretability.

**Interaction Detection and Filtering**

Interaction detection is a critical component of the GAMI-Tree algorithm. It employs an interaction filtering method that assesses the potential of each variable pair to improve model performance through interactions. This process involves identifying significant interactions based on a criterion such as the reduction in prediction error. The filtering is formalized through an algorithm that may use metrics like mutual information or a customized scoring function:

�(�;�)=∑�,��(�,�)log⁡(�(�,�)�(�)�(�))*I*(*X*;*Y*)=∑*x*,*y*​*p*(*x*,*y*)log(*p*(*x*)*p*(*y*)*p*(*x*,*y*)​)

**Iterative Training and Model Refinement**

The iterative approach in GAMI-Tree allows for the sequential refinement of both main effects and interactions:

1. **Initial Fit**: Fit a basic GAM model to capture the main effects.
2. **Boosting Phase**: Sequentially add trees that focus on the residuals of the model, thereby refining the interaction terms.

This iterative refinement ensures the model effectively captures complex relationships within the data while maintaining interpretability.

**Purification of Interactions**

To ensure the model’s interpretability, GAMI-Tree includes a purification step. This step makes the interaction terms hierarchically orthogonal to the main effects, ensuring that they capture unique variance in the data:

���′(��,��)=���(��,��)−Proj��,��(���(��,��))*gjk*′​(*xj*​,*xk*​)=*gjk*​(*xj*​,*xk*​)−Proj*gj*​,*gk*​​(*gjk*​(*xj*​,*xk*​))

Where ProjProj represents the projection of the interaction effect onto the space defined by the main effects.

**Computational Considerations**

The GAMI-Tree algorithm is designed for computational efficiency. It reduces the need for extensive parameter tuning and adapts well to large datasets. The algorithm's performance has been validated through both simulated and real-world datasets, confirming its efficacy and efficiency.

**Conclusion**

GAMI-Tree provides a sophisticated mechanism for fitting interpretable models that can capture both main effects and complex interactions in data. Its structured approach to modeling interactions, combined with the interpretative benefits of GAMs, makes it particularly useful in fields requiring clear explanatory models.

**References**

* Friedman, J. H., & Popescu, B. E. (2008). Predictive learning via rule ensembles. Annals of Applied Statistics, 2(3), 916-954.
* Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013). Accurate intelligible models with pairwise interactions. Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining.
* Tutz, G., & Binder, H. (2006). Generalized additive modeling with implicit variable selection by likelihood-based boosting. Biometrics, 62(4), 961-971.

This detailed technical description provides a comprehensive understanding of the GAMI-Tree algorithm's methodology and mathematical underpinnings, reinforcing its value in statistical modeling and machine learning.

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write a technical explaination on how Explainable boosting machine\ algorithm works. cite journal articles use equations anf formulars

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The Explainable Boosting Machine (EBM) is an advanced machine learning algorithm designed to combine the predictive power of ensemble learning with the interpretability of Generalized Additive Models (GAMs). EBM is essentially an ensemble of GAMs, where each component of the model is a simple shape function that depends on a single feature or a pair of features for interaction terms. Below, I provide a technical explanation of how EBMs work, incorporating mathematical formulations and referencing key journal articles.

**Mathematical Formulation**

EBM is structured around the concept of a generalized additive model with interactions, formalized as follows:

�(�)=�0+∑�=1���(��)+∑�<����(��,��)*f*(*x*)=*β*0​+∑*j*=1*p*​*gj*​(*xj*​)+∑*j*<*k*​*gjk*​(*xj*​,*xk*​)

Where:

* �(�)*f*(*x*) is the predicted outcome.
* �0*β*0​ is the intercept.
* ��(��)*gj*​(*xj*​) represents the contribution of the j-th feature to the prediction, modeled as a function solely of that feature.
* ���(��,��)*gjk*​(*xj*​,*xk*​) are interaction terms modeled as functions of pairs of features.

**Learning Process**

The learning process in EBM involves fitting each component ��(��)*gj*​(*xj*​) and ���(��,��)*gjk*​(*xj*​,*xk*​) sequentially in a boosting-like fashion. Here’s how it generally works:

1. **Initialization**: Start with a constant model, �(0)(�)=�0*g*(0)(*x*)=*β*0​, typically the average of the target values.
2. **Boosting Rounds**: For each feature:
   * Fit a model to the residuals of the previous model.
   * Add this new model to the ensemble, updating the prediction function.

This is repeated for main effects and, optionally, for selected interaction effects.

1. **Cyclic Updates**: Cycle through the features, refining each in turn to improve model accuracy. The update for each feature or interaction term is done using gradient boosting techniques, typically tree-based methods, where each tree is constrained to split only on one feature (or feature pair for interactions).

��(���)(��)=��(���)(��)+�⋅Tree(��)*gj*(*new*)​(*xj*​)=*gj*(*old*)​(*xj*​)+*η*⋅Tree(*xj*​)

Where �*η* is the learning rate, and Tree(��)Tree(*xj*​) is the decision tree fitted to the residuals for feature ��*xj*​.

1. **Regularization**: Regularization techniques such as bagging of trees or shrinking (reducing �*η*) are employed to avoid overfitting.

**Interpretability**

One of the key advantages of EBM is its inherent interpretability:

* **Additive Model**: Since the model is additive, the effect of each feature on the prediction can be individually plotted and understood.
* **Visualization**: The contribution of each ��(��)*gj*​(*xj*​) or ���(��,��)*gjk*​(*xj*​,*xk*​) to the final prediction can be visualized as a function of the feature values, providing clear insights into model behavior.

**Practical Implementation and Performance**

EBMs have been shown to perform comparably to other leading machine learning models while providing significantly better interpretability. They are particularly useful in domains where understanding the model's decision-making process is crucial, such as in finance and healthcare.

**References**

* Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013). Accurate intelligible models with pairwise interactions. Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining.
* Caruana, R., Lou, Y., Gehrke, J., Koch, P., Sturm, M., & Elhadad, N. (2015). Intelligible models for healthcare: Predicting pneumonia risk and hospital 30-day readmission. In Proceedings of the 21st ACM SIGKDD International Conference on Knowledge Discovery and Data Mining (KDD'15).

This description provides an overview of the technical underpinnings of Explainable Boosting Machines, emphasizing both their predictive capabilities and their exceptional transparency.

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The Explainable Boosting Machine (EBM) and GAMI-Tree algorithm both aim to offer interpretable machine learning models that incorporate interaction effects, but they do so using distinct methodologies and techniques. Here, I'll delve into the technical differences between these two algorithms, highlighting their fundamental concepts, mathematical formulations, and how these contribute to their unique characteristics.

**1. Mathematical Formulations**

**Explainable Boosting Machine (EBM)**: EBM is essentially a Generalized Additive Model (GAM) with pairwise interactions, formally represented as: �(�)=�0+∑�=1���(��)+∑�<����(��,��)*f*(*x*)=*β*0​+∑*j*=1*p*​*gj*​(*xj*​)+∑*j*<*k*​*gjk*​(*xj*​,*xk*​)

* �0*β*0​ is the intercept.
* ��(��)*gj*​(*xj*​) are smooth functions representing the effects of individual features.
* ���(��,��)*gjk*​(*xj*​,*xk*​) represent interaction terms between pairs of features.

EBMs iteratively learn each function ��*gj*​ or ���*gjk*​ using boosting techniques, typically employing shallow decision trees that focus on one or two features at a time.

**GAMI-Tree Algorithm**: GAMI-Tree also uses a similar additive model structure but integrates model-based decision trees more deeply into its architecture: �(�)=�0+∑�=1���(��)+∑�<����(��,��)*f*(*x*)=*β*0​+∑*j*=1*p*​*gj*​(*xj*​)+∑*j*<*k*​*gjk*​(*xj*​,*xk*​)

* The key difference lies in the use of model-based trees which optimize a model-fitting criterion at each node, focusing on capturing complex interactions more efficiently.

**2. Learning Approach**

**EBM**:

* Uses a cyclic boosting approach where each feature effect or interaction is learned sequentially.
* Each feature or feature pair is modeled using a series of short decision trees, which are added incrementally to minimize residual errors.
* Regularly cycles back through the features to refine the model incrementally.

**GAMI-Tree**:

* Employs an iterative process that fits model-based trees to the entire dataset, optimizing for interactions from the start.
* Uses advanced interaction detection techniques to prioritize which interactions to model, based on their potential impact on predictive performance.
* Incorporates a "purification" step to ensure the orthogonality of interaction effects relative to main effects.

**3. Interpretability and Visualization**

**EBM**:

* Highly interpretable because each component of the model (both main effects and interactions) can be visualized independently as additive contributions to the model's predictions.
* Allows for straightforward visualization of how each variable and pair of variables affects the outcome.

**GAMI-Tree**:

* Also provides high interpretability with a focus on ensuring that interactions do not contain redundant information from the main effects.
* The purification process helps in clearly distinguishing between the effects of main factors and their interactions, enhancing clarity in model explanations.

**4. Computational Efficiency**

**EBM**:

* Although effective, EBMs can be computationally intensive, especially as the number of features and interactions increases due to its cyclic and sequential boosting approach.

**GAMI-Tree**:

* Tends to be more computationally efficient due to its use of model-based trees, which can capture complex interactions in fewer steps.

**Conclusion**

Both EBM and GAMI-Tree offer robust solutions for building interpretable models capable of incorporating complex interactions. The choice between them may depend on specific needs for model transparency, computational resources, and the particular complexity of the interactions in the dataset.

**References**

* Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013). Accurate intelligible models with pairwise interactions. Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining.
* Hu, L., Chen, J., Nair, V. N., & Mukherjee, A. (2022). Using Model-Based Trees with Boosting to Fit Low-Order Functional ANOVA Models. [Journal Name, Volume, Pages].

These references highlight foundational research and developments in the field of interpretable machine learning, specifically regarding EBM and GAMI-Tree algorithms.

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The Explainable Boosting Machine (EBM) and XGBoost are both powerful machine learning algorithms that are popularly used for supervised learning tasks like classification and regression. However, they differ significantly in their approach, interpretability, and typical use cases. Here's a technical comparison of the two:

**Mathematical Formulations**

**XGBoost**: XGBoost (Extreme Gradient Boosting) operates using the principle of gradient boosting, where many models (typically decision trees) are added one after another to correct the errors made by previous models. The general function for XGBoost can be formulated as: �^�=∑�=1���(��)*y*^​*i*​=∑*k*=1*K*​*fk*​(*xi*​) where:

* �^�*y*^​*i*​ is the prediction for the i-th instance.
* ��*fk*​ are the base learners (trees).
* ��*xi*​ is the feature set for the i-th instance.
* �*K* is the number of boosting rounds/trees.

XGBoost minimizes the following regularized objective: �(�)=∑��(��,�^�)+∑�Ω(��)*L*(*ϕ*)=∑*i*​*l*(*yi*​,*y*^​*i*​)+∑*k*​Ω(*fk*​) where �*l* is a differentiable convex loss function and ΩΩ represents the regularization term which helps in reducing overfitting by penalizing the complexity of the model.

**Explainable Boosting Machine (EBM)**: EBM is a type of Generalized Additive Model (GAM) with interactions, and is represented as: �(�)=�0+∑�=1���(��)+∑�<����(��,��)*f*(*x*)=*β*0​+∑*j*=1*p*​*gj*​(*xj*​)+∑*j*<*k*​*gjk*​(*xj*​,*xk*​) where:

* �0*β*0​ is the intercept.
* ��(��)*gj*​(*xj*​) are smooth functions representing the effects of individual features.
* ���(��,��)*gjk*​(*xj*​,*xk*​) are interaction terms for pairs of features.

EBMs iteratively learn each function ��*gj*​ or ���*gjk*​ using boosting techniques, where each function is modeled using short decision trees or other simple models that focus only on a single feature or feature pair.

**Key Differences**

1. **Interpretability**:
   * **EBM** is designed specifically for interpretability. Each component of the model (main effects and interactions) can be individually examined and visualized, making it straightforward to understand how each feature impacts the model’s predictions.
   * **XGBoost**, while offering feature importance metrics, does not naturally provide a clear, interpretable breakdown of how each feature influences predictions due to its use of complex ensembles of deep trees.
2. **Model Structure**:
   * **EBM** uses an additive model where the impact of features is linearly added, and interactions are explicitly modeled and added as separate terms.
   * **XGBoost** builds an ensemble of trees where each tree can split on any feature, leading to a model where interactions and non-linear relationships are inherently captured but not explicitly modeled for interpretation.
3. **Performance**:
   * **XGBoost** is highly optimized for performance and can handle large datasets efficiently. It is known for winning many Kaggle competitions due to its high performance.
   * **EBM** generally provides competitive accuracy, especially in smaller or medium-sized datasets, with the advantage of being more interpretable.

**References**

* Chen, T., & Guestrin, C. (2016). XGBoost: A Scalable Tree Boosting System. In Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining.
* Lou, Y., Caruana, R., Gehrke, J., & Hooker, G. (2013). Accurate Intelligible Models with Pairwise Interactions. Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining.

This comparison elucidates the fundamental distinctions between EBM and XGBoost, focusing on their core methodologies, advantages, and typical applications.

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