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Evaluating the limitations of gradient boosting and SHAP in predicting magnetite separation performance in PLIMS

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Zhao and colleagues [1] present an enhanced magnetite separation prediction framework that integrates pulsed laser-induced magnetic separation (PLIMS) with multifactor coupling, supervised machine learning, and SHAP-based interpretability. The work addresses the challenge of capturing nonlinear interactions among feed mineralogy, slurry rheology, magnetic flux density, and laser pulse parameters that determine separation efficiency, grade, and recovery.

The methodological approach to predictive modeling in complex, interacting systems warrants consideration of validation strategies appropriate for resource-constrained experimental settings. Unlike clinical ML applications with abundant patient records [2,3], PLIMS data generation involves significant equipment, materials, and time investment per datapoint. Within these constraints, Zhao et al.'s k-fold cross-validation represents a practical approach. To further strengthen validation without excessive resource demands, stratified k-fold cross-validation could ensure representation across operational regimes, and reporting performance variation across folds would provide insight into model stability.

A critical concern regarding Zhao et al.'s approach is the reliance on SHAP for feature importance interpretation. Recent evidence demonstrates that SHAP values, while widely used [4–9], can introduce significant biases, particularly when applied to tree-based models. Bilodeau et al. [16] established formal impossibility theorems revealing fundamental limitations of feature attribution methods like SHAP. Huang and Marques-Silva [17] further documented specific failings of Shapley values for explainability, while Kumar et al. [18] quantified the limitations through Shapley residuals. This concern persists regardless of application domain—whether clinical medicine or engineering. SHAP values are inherently model-dependent (‘explain = SHAP(model)’), potentially amplifying the underlying model's biases rather than revealing true feature relationships [19]. High prediction accuracy does not necessarily guarantee reliable feature importance rankings [20], as tree-based models can exhibit skewed feature importance assessments favoring variables utilized early in tree construction [10,11,21].

While Zhao et al. appropriately connect SHAP interpretations to physical mechanisms, the interpretability could be further strengthened by complementary statistical approaches. Non-parametric methods such as Spearman's rho and Kendall's tau [22] would provide model-agnostic assessments of monotonic relationships between features and separation outcomes. For the complex dependencies and interactions characteristic of PLIMS systems, methods such as Total correlation [23] and Effective transfer entropy [24] could offer valuable insights independent of model architecture. These approaches would require minimal additional computational resources while potentially validating and reinforcing the physics-based interpretations already presented.

We recognize that Zhao et al.'s work represents an important exploratory stage in PLIMS research, where establishing prediction accuracy is the primary goal. The physics-informed feature selection already incorporated in their approach provides a strong foundation. Our recommendations for complementary statistical validation of feature importance would enhance confidence in the identified relationships without requiring additional experimentation.

For future development as the research matures, calibration assessment and operational metrics in physical units (separation efficiency, grade/recovery trade-offs, energy per separated mass) would enhance evaluation of practical utility[12]. These assessments would become particularly valuable when transitioning from exploratory research to implementation planning.

We recommend that Zhao et al. [1] consider enhancing their foundation by: (1) reporting cross-validation performance variation to demonstrate model stability; (2) complementing SHAP analysis with model-agnostic statistical methods to validate feature importance assessments; and (3) where computationally feasible, assessing the stability of key SHAP attributions. This integrated approach would leverage the strengths of both machine learning and statistical analysis, providing more reliable insights into the key factors influencing PLIMS efficiency [13–15].

This balanced methodology acknowledges the realities of resource-intensive engineering research while addressing critical concerns about feature importance interpretation, ultimately leading to more trustworthy insights applicable to magnetite separation optimization.

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Data availability

No data was used for the research described in the article.

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