Multi-objective Evaluation and Optimization of Stochastic Gradient Boosting Machines for Genomic Prediction and Selection in Wheat (*Triticum aestivum*) Breeding

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Abstract

Machine learning (ML) models with stochastic and non-deterministic characteristics are increasingly used for genomic prediction in plant breeding, but evaluation often neglects important aspects like prediction stability and ranking performance. This study addresses this gap by evaluating how two hyperparameters of a Gradient Boosting Machine (GBM), learning rate (v) and boosting rounds (ntrees), impact stability and multi-objective predictive performance for cross-season prediction in a MAGIC wheat population. Using a grid search of 36 parameter combinations, we evaluated four agronomic traits with a comprehensive suite of metrics: Pearsons r, R^2, Area Under the Curve (AUC), Normalized Discounted Cumulative Gain (NDCG), and the Intraclass Correlation Coefficient (ICC) and Fleiss' Kappa for stability. Our findings demonstrate that a low learning rate combined with a high number of boosting rounds substantially improves prediction stability (ICC > 0.98) and selection stability (Fleiss Kappa ≈ 0.90), while also improving generalizability. This combination improved predictive accuracy (r, R^2) and ranking efficiency (NDCG) without a trade-off, though optimal settings were trait-dependent. Conversely, classification accuracy (AUC) was poor and performed relatively better with higher learning rates, revealing a conflict in optimization hyperparameters. Despite low absolute performance for most metrics in the challenging cross-environment prediction, NDCG was high (> 0.85), indicating the models excelled at ranking top-performing entries. This research demonstrates that multi-objective hyperparameter tuning, with a specific focus on stability, is useful for developing reliable genomic prediction models suitable for practical breeding applications.

Introduction

As machine learning (ML) becomes more prevalent in plant breeding, breeders face increasing demands from large genomic and phenotypic datasets, computational time constraints and pressing market and environmental challenges (Pieruschka and Schurr 2019; van Dijk et al. 2020; Calvin et al. 2023; Yoosefzadeh Najafabadi et al. 2023; Crossa et al. 2025). The effectiveness of ML models depends on how they are constructed, optimized, and evaluated (Domingos 2012; Feurer and Hutter 2019). Model evaluation often relies on a limited range of metrics emphasizing overall predictive accuracy, via Pearson's correlation (r) or Coefficient of Determination (R^2) (Meuwissen et al. 2001; Goddard and Hayes 2007). Although overall predictive accuracy is fundamental to assessing model performance, relying solely on accuracy metrics to evaluate ranking efficiency, selection efficiency, and stability, is inherently limited; this creates an evaluation gap in breeding programs and underscores the need for targeted metrics (Blondel et al. 2015; Dekkers et al. 2021; Lange et al. 2025).

A multi-metric evaluation is therefore justified to address this gap. Ranking ability can be assessed with Normalized Discounted Cumulative Gain (NDCG), which rewards the correct ordering of top-performing candidates (Järvelin and Kekäläinen 2002; Blondel et al. 2015). For binary "select/reject" decisions, the Area Under the Curve (AUC) measures a model's ability to distinguish between classes (Huang and Ling 2005; Robin et al. 2011). Yet, neither metric directly addresses the issue of non-determinism, or stochasticity, inherent in many algorithms.

In stochastic Gradient Boosting Machines (GBM), random subsampling introduces variability between runs (Friedman 2002). This requires explicit stability assessment. The Intraclass

Correlation Coefficient (ICC) can quantify the consistency of continuous predictions across iterations (Bartko 1966; McGraw and Wong 1996; Weir 2005; Koo and Li 2016; Lange et al. 2025). A high ICC value indicates that variability in predictions is mainly due to inherent differences among targets rather than random fluctuations, demonstrating stable model performance (Weir 2005). For categorical selections, Fleiss kappa (κ) measures the stability of agreement among "candidate" classifications across runs (Fleiss 1971; Lange et al. 2025).

GBM performance is influenced by hyperparameters that balance the bias-variance trade-off. The learning rate and the number of boosting rounds must be carefully tuned to capture data complexity without overfitting (Friedman 2001; Ridgeway and Developers 2003). This creates a multi-objective optimization problem: maximizing predictive, selection and ranking accuracy while ensuring high stability.

This study performs a parametric optimization of a stochastic GBM to address these challenges. We systematically evaluate 36 combinations of learning rate and boosting rounds using genomic and phenotypic data from a Multi-parent Advanced Generation Inter-Cross (MAGIC) wheat population. Cross-season predictions are assessed on four traits-Grain Yield (GY), Grain Protein Content (GPC), Thousand Grain Weight (TGW), and Height to Ear tip (HET). We aim to: (1) evaluate performance using Pearson's r, R^2, NDCG, and AUC; (2) quantify prediction and selection stability with ICC and Fleiss κ; (3) determine the effects of hyperparameters on all metrics; and (4) provide insights into model generalizability. Findings will help breeders select ML models that are not only accurate but also stable enough to support confident, repeatable selection decisions.

Methods and Materials

A 500-line wheat (*Triticum aestivum*) Multi-parent Advanced Generation Inter-Cross (MAGIC) population was analyzed (Scott et al. 2021). Four agronomic traits were assessed from their study: GY, TGW, GPC, HET in a cross-season prediction scenario. Field experiments were conducted at Girton, UK (52.24144 °N, 0.08794 °E; 2016-17 season, training) and Whittlesford, UK (52.09909 °N, 0.13311 °E; 2017-18 season, testing) (Scott et al. 2021).

SNP genotyping and quality control

Genotypes comprised 25,508 single-nucleotide polymorphisms (SNPs) from the Axiom 35k wheat breeders' SNP genotyping array (Winfield et al. 2016). Loci with > 5 % missing calls were excluded. Remaining missing values were imputed by Random Forest using the missRanger R package (v2.5.0, see S1 - Package_Functions) (Mayer 2024).

Train-test splits

To evaluate performance in a cross-environment prediction scenario, models were trained using data from the 2016/17 season and evaluated against observed phenotypes from the 2017/18 season. Five random 80%/20% partitions of the 500 lines were generated using set.seed(123).

Gradient-boosting

Stochastic gradient-boosting machine was fitted with gbm v2.2.2 in R 4.4.3. A 6 × 6 crossed tune grid, learning rate = {0.0025, 0.042, 0.0815, 0.121, 0.1605, 0.20} with boosting rounds = {100, 1080, 2060, 3040, 4020, 5000}, while all other arguments remained at default (including bag.fraction = 0.5) (S1 - Package_Functions). (DOI: 10.5281/zenodo.15829464 - Data Availability).

The ensemble update at boost round m followed (Friedman 2002; Ridgeway and Developers 2003):

$$F_m(x) = F_{m-1}(x) + \nu \rho_m h(x; a_m)$$

Where:

$F_m(x)$ is the updated ensemble prediction

$F_{m-1}(x)$ is the prediction from the previous iteration

ρ_m is the optimal step length determined via line search

$h(x: a_m)$ is a regression tree fit to the pseudo residuals

ν is the learning rate (shrinkage, $0 < \nu \leq 1$)

Prediction pipeline

For each of the five train-test splits, each of the ten stochastic model fits was independently used to generate predictions on its corresponding 20% hold-out set. This yielded 50 distinct prediction vectors (5 splits × 10 iterations per split) for each hyperparameter combination, which were then compared to the observed phenotypes. Reproducibility ensured via set.seed(123 + split_number × 1000 + prediction_iteration) (DOI: 10.5281/zenodo.15829464 - Data Availability). See Fig. S1 for prediction to evaluation pipeline flowchart.

Performance and stability metrics

Performance metrics, Accuracy - Pearsons correlation (r) and coefficient of determination (R^2) - and ranking efficiency - Normalized Discounted Cumulative Gain at the top 20 % (NDCG@20 %), and classification ability - by labeling lines with observed phenotypes above the 75th percentile as Candidates and then computing the ROC AUC (File S1 - Formulae). Stability across the ten stochastic repeats was quantified by the single-measure, one-way intraclass correlation coefficient (ICC) for predictions and by Fleiss κ for overall agreement of binary

selection (File S1 - Formulae, DOI: 10.5281/zenodo.15829464 - Data Availability). Across the hyperparameter grid, each trait yielded n = 1,800 performance estimates (r, R^2, NDCG@20 %, AUC; 5 splits × 6 learning-rates × 6 boost-rounds 10 iterations) and n = 180 stability estimates (ICC, Fleiss K; 5 splits × 6 learning-rates × 6 boost-rounds) (File S4).

Data visualization

Figures were generated with ggplot2 3.4 and viridis 0.6. Error bars are the standard error (± SE) which are found in the table of summary statistics (mean, SD, SE, min, max, IQR) for every metric and hyperparameter combination in File S2. Min-max normalization of performance and stability metrics were applied and plotted as supplementary material (Fig. S2).

Statistical analysis

All statistics were run in R 4.4.3 to quantify how GBM hyperparameters influence predictive performance and stability within and across traits. Normality of predicted values was screened with Shapiro-Wilk tests. Q-Q and residual-versus-fitted plots were made for observing normality of residuals (Fig. S4).

Modelling framework

Trait-wise predictive performance was analyzed with random-intercept linear mixed-effects models (LMM; lme4 1.1-36), using learning rate and boosting rounds as fixed effects and random intercepts to account for Subset and Subset:Iteration nesting. Trait-wise stability was assessed non-parametrically via Friedman tests (friedman.test(Value ~ ParameterLabel | Subset)). To examine hyperparameter effects across traits, we fitted three-way LMMs (Trait × Learning Rate × Boost Rounds) with random intercepts for Trait and Subset (and, for performance only,

Subset:Iteration). Cross-trait (aggregated) performance and stability were evaluated with two-way LMMs (Learning Rate × Boost Rounds), where performance models again included Subset:Iteration, but stability models retained only Trait and Subset nesting. Fixed effects were tested by Satterthwaite-approximated F-tests (lmerTest 3.1-3), Tukey-adjusted pairwise tests were made via emmeans 1.11.0. All p-values reported are raw unless otherwise specified, with post-hoc contrasts presented as Tukey-adjusted p-values. (DOI: 10.5281/zenodo.15829464 - Data Availability, File S3).

Results

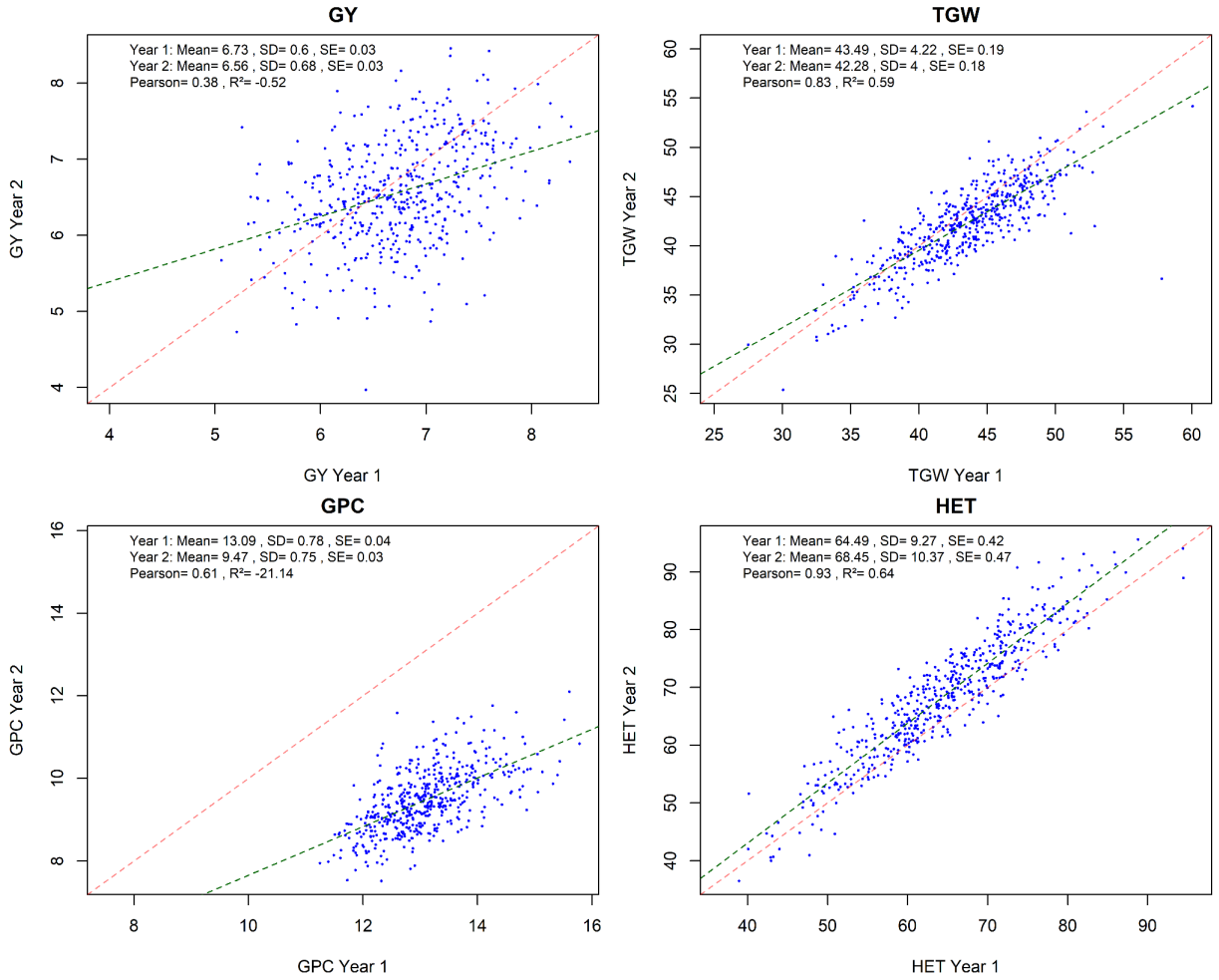

Figure 1. This figure displays four scatter plots, showing the relationship between Year 1 (x-axis) and Year 2 (y-axis) observed measurements for four agronomic traits from the wheat dataset. Traits: GY (grain yield) - top left, TGW (thousand grain weight) - top right, GPC (grain protein content) - bottom left and HET (height to ear tip) - bottom right. Each blue point represents an individual wheat line's measurements in both years. The red diagonal line is the 45° identity line, indicating (theoretical) perfect agreement between the two years. The green dashed line is the best-fit regression line. The annotations in each panel summarize the mean, standard deviation (SD), and standard error (SE) for both years, along with the Pearson correlation coefficient and the coefficient of determination (R^2).

Analysis of raw agronomic data of the 500 entries across two seasons found that some traits were more stable year-to-year than others. TGW and HET showed strong Pearson correlations between years (r = 0.83 and r = 0.93, respectively). In contrast, GY showed a weak cross-year correlation (r = 0.38), whereas GPC was moderate (r = 0.61). The mean values for GPC also varied largely between the first year (13.09% SE = 0.03) and the second year (9.47% SE = 0.03), unlike other traits (Fig. 1).

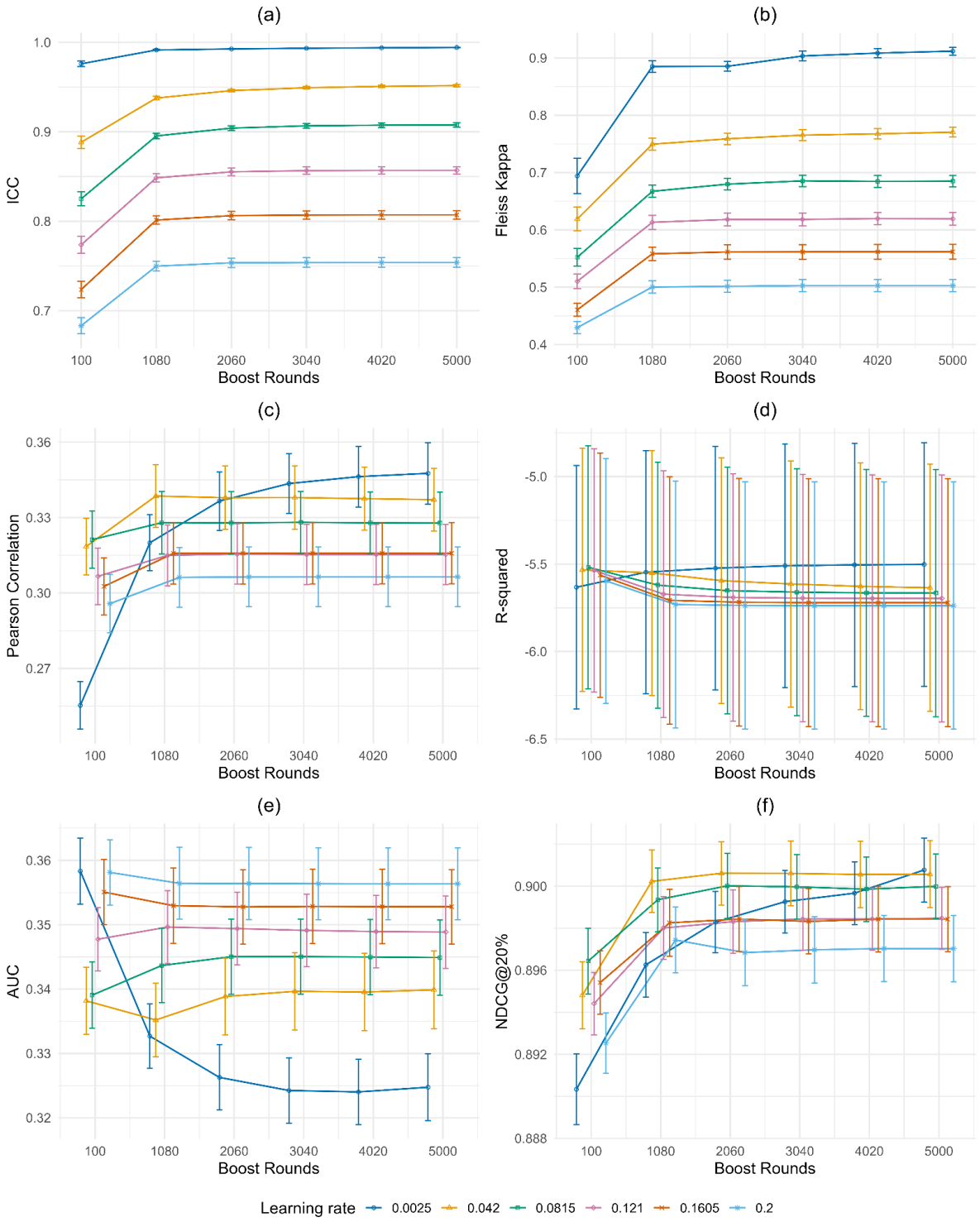

Figure 2. Displays trait aggregated values for six performance metrics: Intra-class Correlation Coefficient (ICC, top left), Fleiss' Kappa (top right), Pearson Correlation (middle left), R2 (middle right), Area Under the Curve (AUC, bottom left), and Normalized Discounted Cumulative Gain at the top 20% ranking (NDCG@20%, bottom right). Each plot shows aggregated results across all four traits, with the x-axis representing boosting rounds and the y-axis indicating the respective evaluation metric. Colored lines connect the mean metric values for each learning rate, and error bars reflect ±1 standard error. This figure provides a view of model performance across all metrics. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

To determine the optimal hyperparameters for genomic prediction, we evaluated the effects of learning rate and boosting rounds on overall model performance and stability by analyzing metrics aggregated across all four traits. Elapsed time was not affected by learning rate but increased linearly with boosting rounds: models with 100 rounds finished in under 30 minutes per core, while 5,000 boost rounds required ≈10 hours per core (Fig. S3).

The aggregated performance of the 36 hyperparameter combinations across all traits is presented in Figure 2. Models combining low learning rates (v = 0.0025 - 0.0815) with moderate-to-high boosting rounds (> 2 000) achieved the highest Pearson correlation, R^2, and NDCG@20% (Fig. 2a-d, 2f). There was no observable trade-off between predictive accuracy (r and R^2) and ranking performance (NDCG@20 %) while marked improvements in stability metrics (ICC and Fleiss Kappa) were observed (Fig. 2a-d, 2f). A three-way ANOVA, with fixed-effect significance determined by Satterthwaite-approximated F-tests, revealed that the interaction of trait × learning rate × boosting rounds was a significant source of variation for all four performance metrics: Pearson correlation, R^2, AUC, and NDCG@20% (e.g. Pearson: $F_{(3, 6988)} = 44.79$, $p < 0.001$ for all). This indicates that optimal hyperparameter settings were trait-dependent. The two-way interaction between learning rate × boosting rounds was also significant across all four metrics (e.g. R^2: $F_{(1, 6988)} = 105.14$, $p < 0.001$). Full ANOVA results are available in File S3.

Pairwise comparisons of the estimated marginal means (Tukey-adjusted) for the aggregated results identified two distinct performance trends. For Pearson correlation, R^2, and NDCG@20%, models with lower learning rates (v = 0.0025 - 0.0815) combined with a moderate-to-high number of boosting rounds (ntrees > 2,000) significantly outperformed models with higher learning rates ($p < 0.001$) (Fig. 2c, 2d, 2f). In contrast, classification accuracy (AUC)

followed an opposite trend. Models with higher learning rates consistently and significantly outperformed those with lower learning rates across all boosting round counts ($p < 0.001$) (Fig. 2e).

While the interactions were significant, the main effects of the hyperparameters varied by metric. For Pearson correlation and NDCG@20%, the main effect of learning rate alone was not significant ($p = 0.566$ and $p = 0.210$, respectively). For R^2, the main effect of boosting rounds was not significant ($p = 0.720$). In contrast, boosting rounds showed a strong main effect on Pearson correlation ($F_{(1, 6\,988)} = 319.73$, $p < 0.001$), whereas learning rate had a significant main effect on R^2 ($F_{(1, 6\,988)} = 87.76$, $p < 0.001$). The aggregated trait R^2 values showed high uncertainty, as shown by the standard error bars in Figure 2d and 4c (see Figure S2d for min-max normalization).

The effect of hyperparameter tuning on model stability revealed a critical difference between the two metrics evaluated (Figure 2a, 2b). A three-way ANOVA found that the trait × learning rate × boosting rounds interaction was not significant for the Intraclass Correlation Coefficient (ICC) (($F_{(3, 688)} = 0.11$, $p = 0.957$), indicating that the effect of tuning on prediction stability was consistent across traits. In contrast, this three-way interaction was significant for Fleiss Kappa ($F_{(3, 688)} = 4.72$, $p < 0.001$), showing that optimal settings for selection stability were trait-dependent (File S3 - ANOVA 3-way).

Despite this difference, the main effect of learning rate was highly significant for both stability metrics (e.g. ICC: $F_{(1, 688)} = 3398.53$, $p < 0.001$), confirming its primary role in improving stability. Full ANOVA results are available in Supplementary File S3 - ANOVA 3-way.

Pairwise comparisons of the estimated marginal means (Tukey-adjusted) confirmed a unified trend: lower learning rates produced significantly higher stability scores for both ICC and Fleiss' Kappa, with nearly all learning rate combinations being significantly different from one another when compared at similar boosting round levels ($p < 0.001$; see File S3).

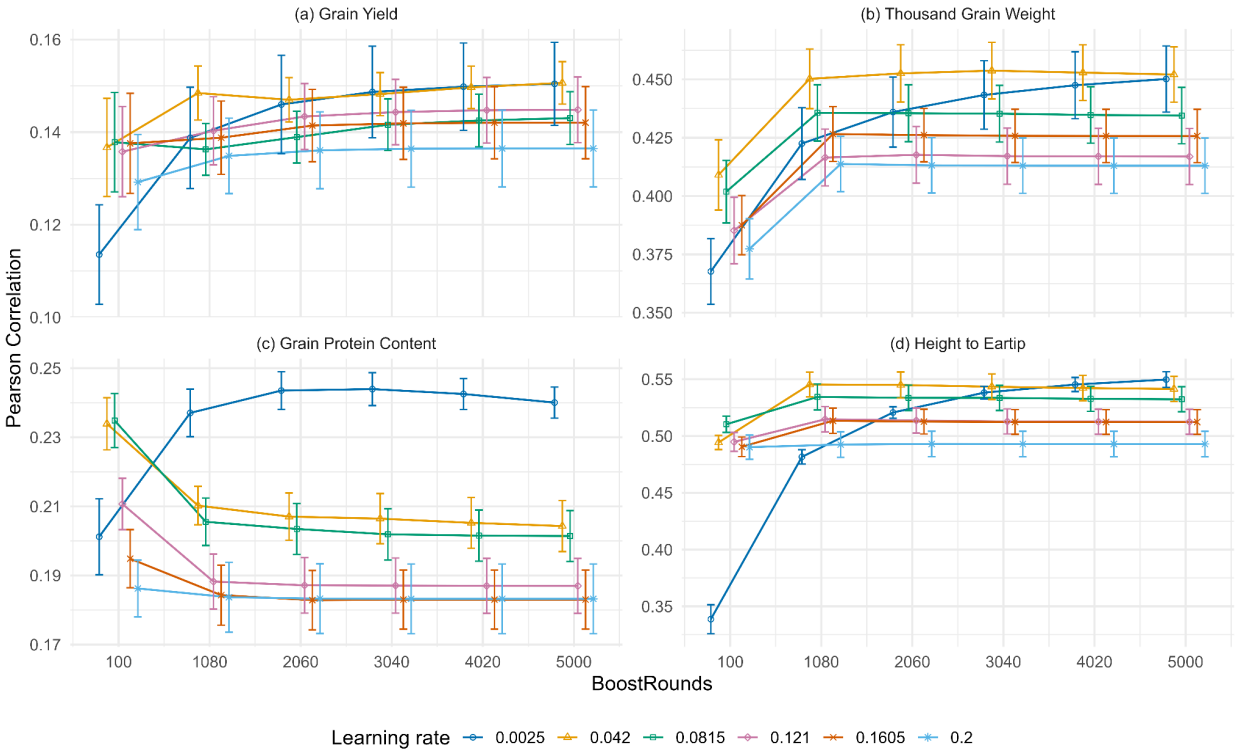

Figure 3. Displays the Pearson correlation coefficient varies with boosting rounds and learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left) , Height to Ear Tip (HET - bottom right). The x-axis represents boosting rounds and the y-axis indicates the mean Pearson correlation for each model combination, with error bars showing ±1 standard error. Coloured lines connect mean values for each learning rate. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

Absolute predictive performance for Pearson correlation varied by trait. GPC showed the greatest increase in Pearson correlation at an intermediate number of boosting rounds when using learning rate v = 0.0025 (Fig. 3c). The mean Pearson r across hyperparameter combinations was 0.42 (SD 0.091) for TGW and 0.51 (SD 0.080) for HET (Fig. 3a-d, File S5). A two-way ANOVA for each trait showed that the interaction between learning rate × boosting rounds was significant for GY ($p < 0.05$), TGW ($p < 0.001$), and HET ($p < 0.001$). The main effects also

varied: boosting rounds was a significant factor for GY, TGW, and HET ($p < 0.001$), while learning rate was significant for TGW, GPC, and HET ($p < 0.05$). Full ANOVA results for each trait are available in File S3 - ANOVA Trait Specific 2-way.

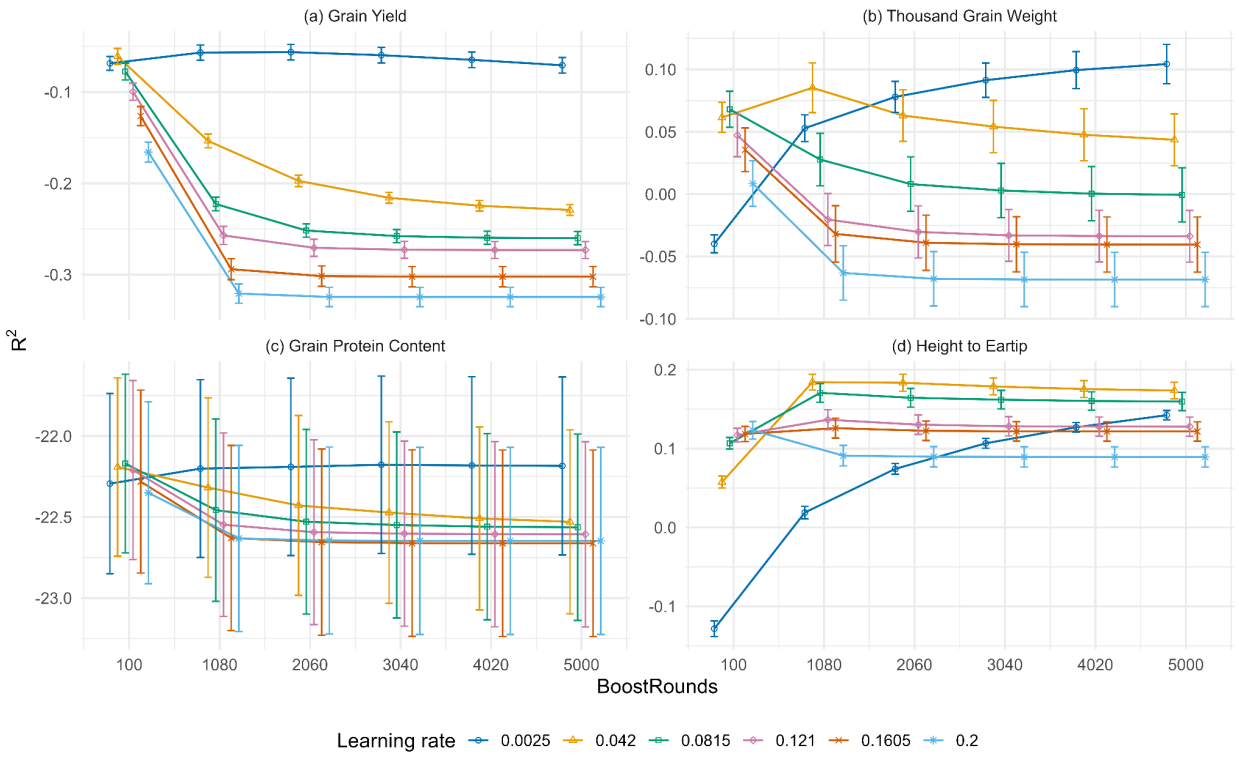

Figure 4. The plot shows Correlation Coefficient of Determination (R2) relationship with boosting rounds by learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left), Height to Ear Tip (HET - bottom right). The x-axis represents boosting rounds and the y-axis indicates the mean R2 for each model combination, with error bars showing ±1 standard error. Faceted plots have free y-axis scales. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

Model performance as measured by R^2 was poor, with values for GY and GPC being consistently negative (Fig. 4a, 4c). R^2 for GPC was also characterized by extremely low absolute value, high variability and uncertainty ($R^2 < -21$, SD = 3.96, SE = 0.09, File S5). A high uncertainty in R^2 for GPC obscured performance differences among the hyperparameter combinations (Fig. 4c). In contrast, R^2 values for TGW and HET were mostly positive though low (Fig. 4b, 4d).

A two-way ANOVA for each trait confirmed that the main effects of learning rate and boosting rounds, as well as their learning rate × boosting rounds interaction, were significant for all four traits ($p < 0.001$ for all). The nature of this interaction showed that for the lowest learning rate ($v = 0.0025$), R^2 values generally increased with more boosting rounds. Conversely, for higher learning rates ($v \geq 0.042$), R^2 values tended to decrease as boosting rounds increased (Fig. 4). Full ANOVA results are available in File S3 - ANOVA Trait Specific 2-way.

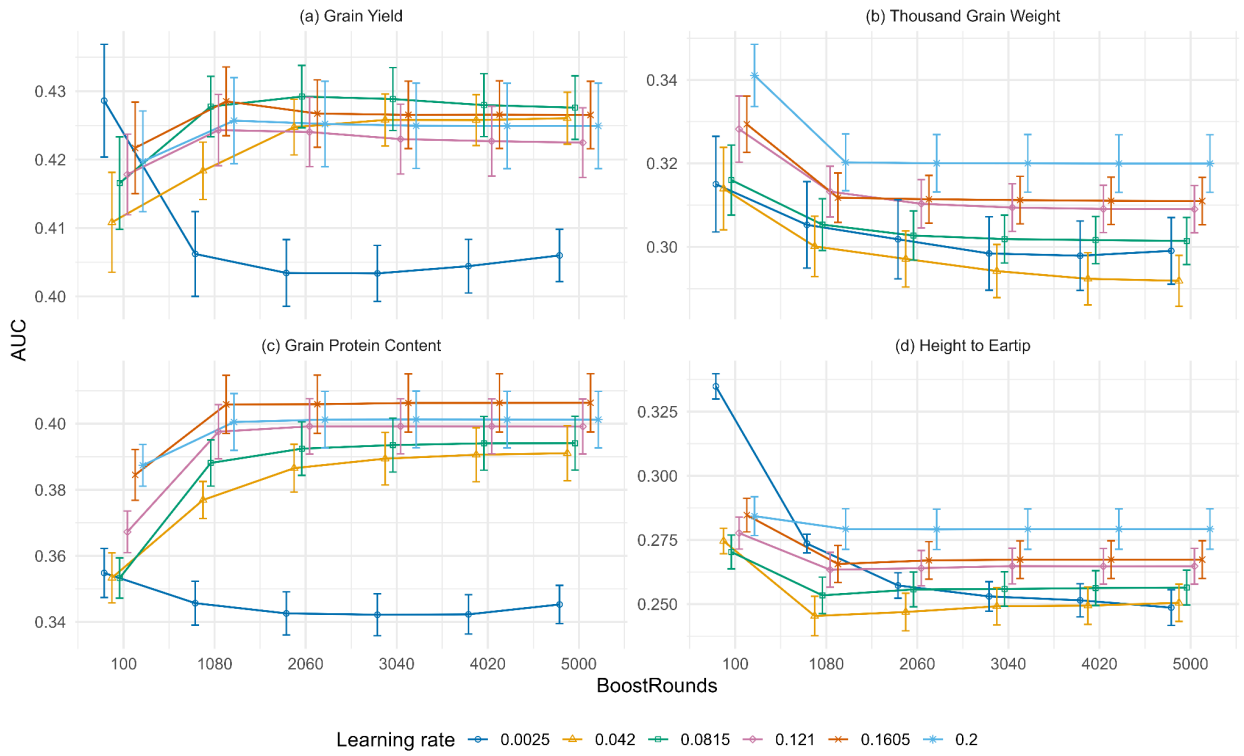

Figure 5. Displays Area Under the Curve (AUC) by boosting rounds across learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left) , Height to Ear Tip (HET - bottom right). The x-axis represents boosting rounds and the y-axis indicates the mean AUC for each model combination, with error bars showing ±1 standard error. Colored lines connect mean values for each learning rate. Data are presented in separate panels for each trait with free y-axis scales. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

Classification accuracy, measured by Area Under the Curve (AUC), was poor across all hyperparameter combinations, with values below the 0.5 threshold of random chance for all four traits (Fig. 5a-d). Visually, models with higher learning rates ($v \geq 0.042$) generally resulted in higher AUC values, often peaking with 1000 - 2000 boosting rounds. In contrast, the lowest

learning rate (v = 0.0025) consistently produced lower AUC values across all boosting rounds. With a learning rate of v = 0.0025, AUC decreased during moderate-to-high numbers of boosting rounds but began to increase from 4,000 boost rounds.

A two-way ANOVA for each trait showed that the main effect of learning rate was significant for all four traits ($p < 0.05$). The main effect of boosting rounds was significant for TGW, GPC, and HET ($p < 0.05$), but not for GY. Notably, the learning rate × boosting rounds interaction was only significant for HET ($p < 0.001$). ANOVA results are available in File S3 - ANOVA Trait Specific 2-way.

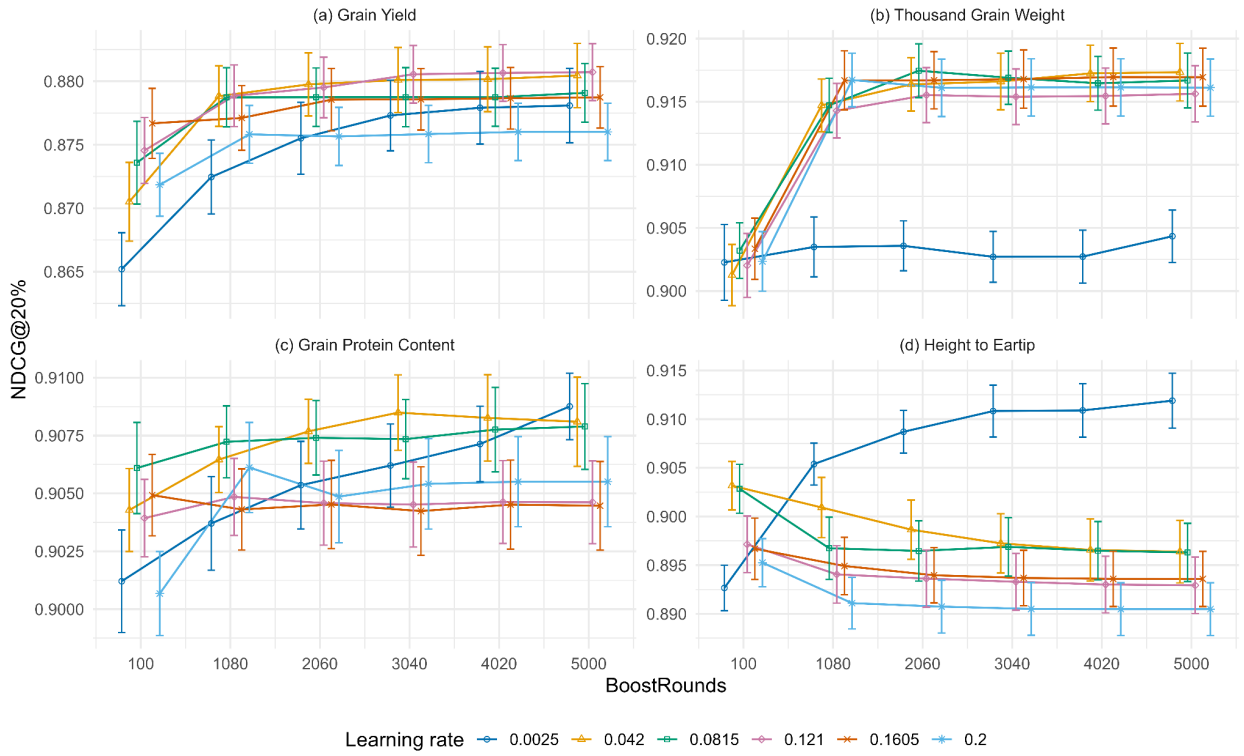

Figure 6. The plot displays Normalized Discounted Cumulative Gain (NDCG) evaluated at the cutoff corresponding to the top 20% position of ranked entries (denoted, NDCG@20%) compared to different combinations of boosting rounds and learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left) , Height to Ear Tip (HET - bottom right). The x-axis shows boosting rounds and the y-axis indicates the mean NDCG@20% for each model combination, with error bars showing ±1 standard error. Colored lines connect mean values for each learning rate. Data are presented in separate panels for each trait with free y-axis scales. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

Ranking performance, measured by NDCG@20%, was high across all traits, with values consistently above 0.85 (Fig. 6, File S2, S4). A two-way ANOVA for each trait showed that the main effects of learning rate and boosting rounds, as well as their interaction, were significant for GY, TGW, and HET ($p < 0.05$). For GPC, the main effect of learning rate was not significant ($p = 0.82$), although boosting rounds and the interaction remained significant ($p < 0.05$). Figure 6 shows that for the lowest learning rate ($v = 0.0025$), NDCG@20% values generally increased across all boosting rounds. In contrast, for higher learning rates, performance typically peaked with 1000-3000 boosting rounds before plateauing or declining (Fig. 6a-d). Full ANOVA results are available in File S3 - ANOVA Trait Specific 2-way.

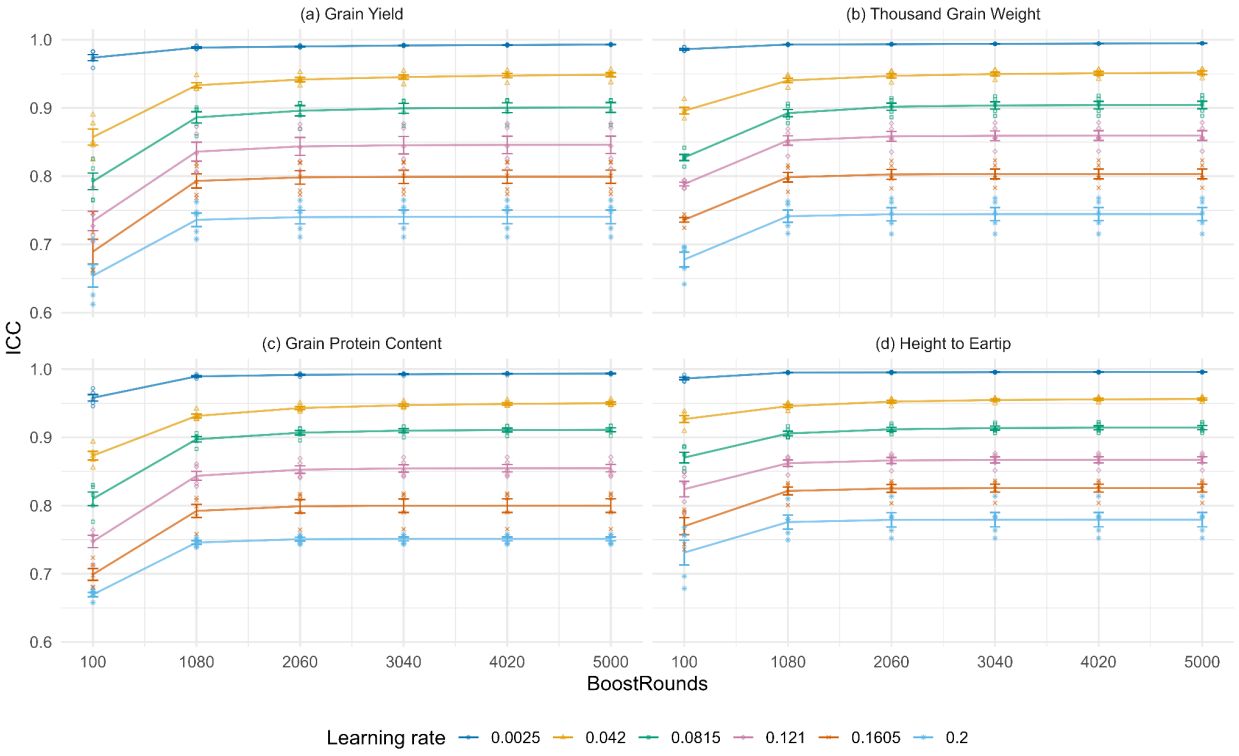

Figure 7. The plot displays the intra class correlation coefficient (ICC) compared to combinations of boost rounds and learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left) , Height to Ear Tip (HET - bottom right). The x-axis represents boost rounds and the y-axis shows ICC. For each trait and learning rate, mean ICC values are connected by dashed lines with error bars indicating ±1 standard error. Individual ICC observations appear as points. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

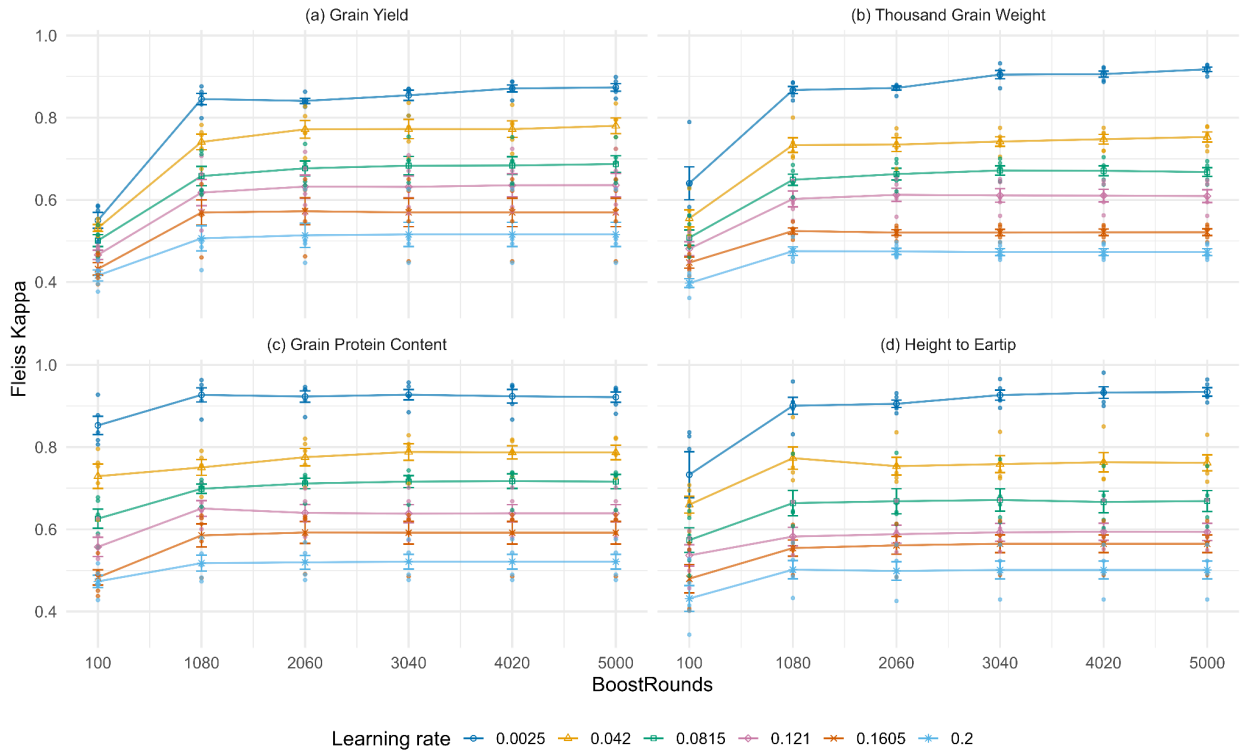

Figure 8. The plot displays the Fleiss' Kappa compared to combinations of boost rounds and learning rate across four traits Grain Yield (GY - top left), Thousand Grain Weight (TGW - top right), Grain Protein Content (GPC - bottom left) , Height to Ear Tip (HET - bottom right).. The x-axis represents boost rounds and the y-axis shows ICC. For each trait and learning rate, mean Fleiss' Kappa values are connected by dashed lines with error bars indicating ±1 standard error. Individual Fleiss' Kappa observations appear as points. Each color corresponds to a distinct Learning Rate; Dark Blue (0.0025), Orange (0.042), Green (0.0815), Purple (0.121), Red-Orange (0.1605), and Light Blue (0.2).

Prediction stability (ICC) and selection stability (Fleiss Kappa) showed highly consistent and clear trends across all four traits (Fig. 7, 8). For both metrics, stability values systematically increased as the learning rate decreased. The lowest learning rate ($\nu = 0.0025$) consistently resulted in the highest stability, with ICC values approaching 1.0 for all traits at 5,000 boost rounds ($M = 0.994$, $SD = 0.001$, $N = 20$; File S4, S2). For any given learning rate, stability also increased with more boosting rounds, typically plateauing after approximately 2,000 rounds (Fig. 7, 8). For each trait, significant differences among the 36 hyperparameter combinations were confirmed for both ICC and Fleiss' Kappa (Friedman test, $p < 0.001$, File S3 - Trait Specific Friedman Stab.).

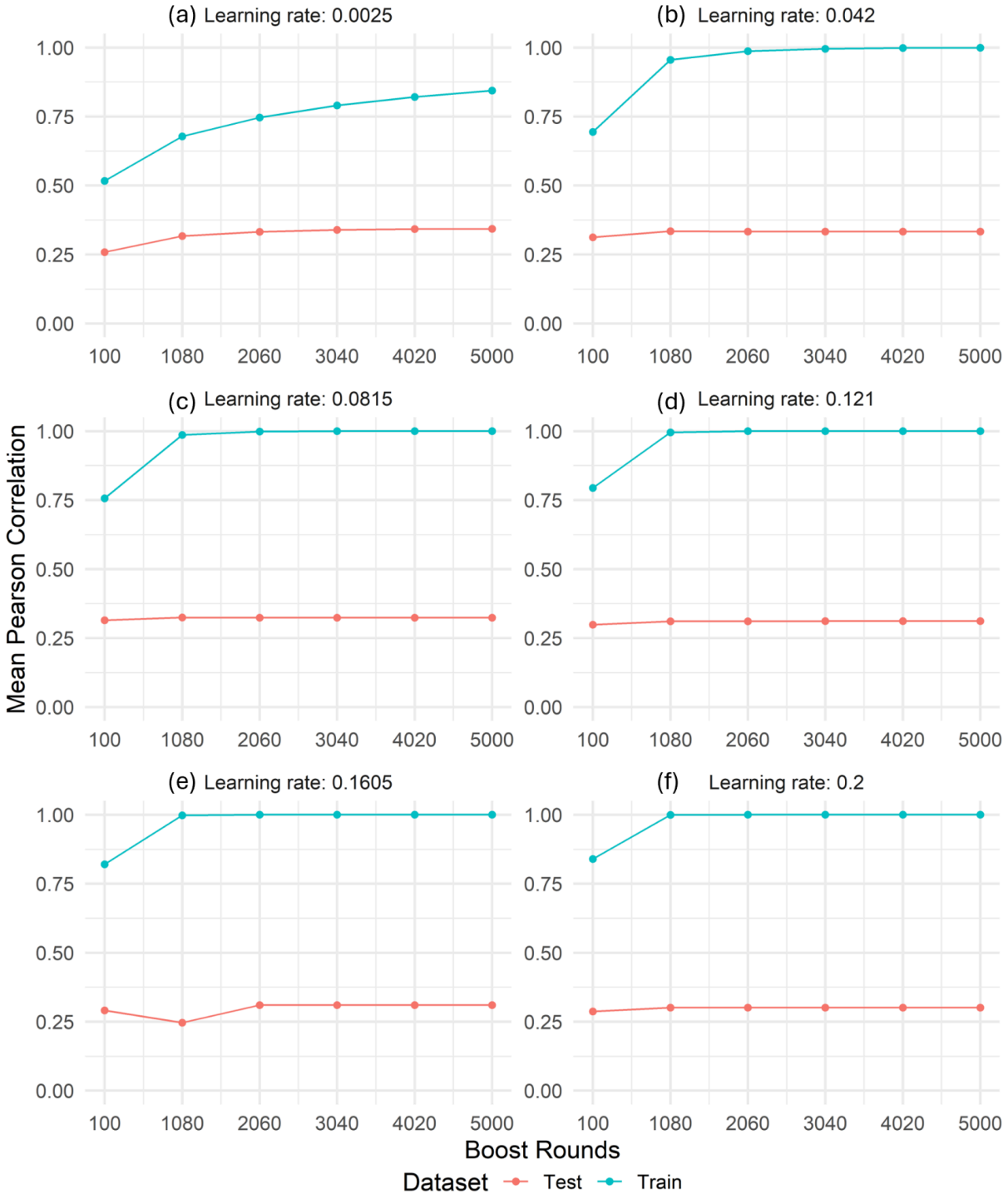

Figure 9. Shows the relationship between correlation coefficient and boosting rounds across different learning rates with traits aggregated. The y-axis shows the mean Pearson correlation coefficient. The x-axis shows the number of boosting rounds. Each facet represents a different learning rate. In each plot, the blue line depicts model performance on the training data, while the orange-red line shows performance on unseen test data, allowing the visualization of overfitting.

Model generalizability was assessed by comparing the mean Pearson correlation on the training and test datasets for each learning rate across boosting rounds (Figure 9a-f). A performance gap was observed for all hyperparameter combinations, with training set correlations consistently higher than test set correlations. For learning rates of 0.042 and higher, training performance rapidly approached a correlation of 1.0, creating a large gap relative to the test performance (Fig. 9b-f). In contrast, for the lowest learning rate (v = 0.0025), training performance increased more gradually, resulting in the smallest performance gap between the training and test datasets among all tested learning rates (Fig. 9a).

Discussion

The stochastic characteristic of many modern genomic prediction models produce stochastic outputs; evaluating them solely on predictive accuracy ignores this critical instability and undermines their reliability for making consistent selection and ranking decisions in breeding programs. Our multi-objective hyperparameter search addresses this gap, revealing that prioritizing model stability (via ICC and Fleiss' Kappa) is a highly effective strategy. A configuration with a low learning rate and a high number of boosting rounds raised prediction stability to near-deterministic levels, while also providing significant concurrent improvements in predictive (r, R^2) and ranking (NDCG) performance. While hyperparameters optimized for stability metrics were consistent across traits, performance metrics benefitted from trait-specific configurations. This complexity underscores the necessity of a multi-objective approach, as no single optimization strategy can meet all the diverse objectives within breeding programs.

The use of low learning rates increased prediction stability to substantial, near-deterministic levels (ICC > 0.98), providing breeders with more consistent predictions (Fig. 2a, 7). According to the Landis & Koch (1977) scale, as revised (1998), ICC values > 0.80 indicate substantial reliability (Shrout 1998). Low learning rates also significantly improved the consistency of selection classifications from fair to excellent (Fleiss' Kappa > 0.8), ensuring the classification of predicted candidates remains stable. For context, the framework for Fleiss Kappa defines agreement above ~0.75 as excellent (Fleiss 1971).

Our aggregated trait analysis identified an optimal configuration across the 36 evaluated hyperparameter combinations: a very low learning rate (v = 0.0025) combined with a high number of boosting rounds (ntrees = 5000) achieved the highest combined stability, predictive accuracy, and ranking efficiency (Friedman 2002). However, a window of models, specifically those with low learning rates (e.g., v ≤ 0.042) and boosting rounds exceeding 2,000 offered statistically similar performance for accuracy and ranking metrics. This suggests smaller models with low learning rates can achieve similar performance with substantially less computation (Friedman 2002).

In contrast to other metrics, classification accuracy (AUC) revealed a conflict in optimization objectives: it not only performed worse than random chance across all models and traits but also favored a different hyperparameter configuration, where fewer boosting rounds and higher learning rates yielded better relative discriminatory ability. A study reported similar optimal hyperparameters for their gradient boosting model (XGBoost) using AUC, found their models performed best at their tested maximum of 100 boost rounds and a learning rate of 0.01 - 0.1

(Jeon et al. 2024). Since the total AUC metric evaluates performance across all decision thresholds, it can obscure a model's utility for breeders by giving undue weight to irrelevant portions of the ROC curve (Bradley 1997; Peng et al. 2024). We therefore support that a partial AUC (pAUC), by restricting the analysis to a relevant window of high True Positive and low-to-moderate False Positive Rates (TPR, FPR), should be explored for a more relevant metric for gauging the discriminatory power of models for candidate selection (McClish 1989; Peng et al. 2024). Our findings suggest that model optimization requires a strategic choice based on the primary objective, allowable tradeoffs and trait of interest, as a single set of hyperparameters could not deliver optimal performance across all evaluation metrics. The poor absolute values for AUC are likely a plausible consequence of the challenging cross-environment scenario where candidate assignment was based on the top 25% of observed phenotypes within the test environment, creating a 'moving target' with an arbitrary upper threshold. The unmodeled environmental covariates were likely an important factor in the poor cross-environment prediction. The absence of these covariates inhibited the modeling of G × E interactions, which can degrade the cross-season performance (Jarquín 2017; Tomar et al. 2021; Montesinos-López et al. 2022).

Despite the model's low absolute prediction and classification accuracy, its strong ranking performance (NDCG@20% > 0.85) demonstrates its practical utility for elite-line discovery, where correctly selecting or ranking top candidates is more valuable than predicting their exact performances. This high ranking performance, in contrast to the lower Pearson r and R^2 values, is explained by the nature of the NDCG metric, which focuses specifically on rewarding the correct ordering of top-performing entries rather than penalizing errors across the entire distribution

(Blondel et al. 2015; Pan et al. 2024). The suitability of this metric for breeding decisions, where correctly ranking and selecting elite lines is a primary goal, has led to its increasing adoption (Gianola et al. 2018; Negussie et al. 2022; Li et al. 2023; Pan et al. 2024).

The ANOVA results confirm that model performance is influenced mostly by main effects of learning rate and boosting rounds but also by their significant interaction, which supports the need for co-optimization. This hierarchy of effects is consistent with previous research where learning rate was as a dominant hyperparameter for XGBoost model with a general support for lower learning rates (Westhues et al. 2021). The learning rate provides regularization that prevents overfitting to subsample artifacts by shrinking the contribution of each new boost round (Elith et al. 2008). The non-significant three-way interaction for prediction stability (ICC) is an important result as it indicates that the relationship between learning rate and boosting rounds was consistent across all traits, suggesting that an optimized hyperparameter combination for stability may be broadly applicable across traits.

An important finding was the trait-specific response to hyperparameter tuning. While the overall pattern (favoring low learning rates and high boost rounds) was consistent, the magnitude of improvement and the optimal settings varied by trait. For example, the strong response of GPC to a very low learning rate suggests its genetic architecture is likely controlled by many small-effect loci, which are captured, more effectively, through larger models that learn slowly(Azodi et al. 2019; Sandhu et al. 2021; Paina and Gregersen 2023). In contrast, for HET, the benefit of low learning rates was less clear. This variation in optimal settings between traits

underlines the need for trait specific parameter optimization to best model the distinct genetic architecture of each trait (Azodi et al. 2019; Zingaretti et al. 2020).

While our results demonstrate the benefits of GBM hyperparameter tuning for genomic prediction, we acknowledge the limitations of this study. First, the overall performance metrics, Pearson, R^2, and AUC, remained low-moderate in absolute terms across all quantitative traits. This poor performance is supported by a clear train-test gap, suggesting overfitting. Across 36 GBM settings, at $\approx$ 1000 boosting rounds, Pearson r on the training data (16/17) approached unity ($r \approx 1.0$) for every learning rate except $v = 0.0025$, while Pearson r on the test data (17/18) remained low. The $v = 0.0025$ model produced the smallest train-test gap. This result aligns with established principles, confirming that learning rates are useful for maintaining generalizability and mitigating overfitting (Friedman 2001; Elith et al. 2008).

Training (Girton 2016/17, clay-loam) and test (Whittlesford 2017/18, loam) sites differed in soil, management and season, yet no environmental covariates or multi-environment-trial (MET) terms were added to the model. The inclusion of MET data presents an opportunity to improve model performance, as including environmental covariates has been shown to benefit generalizability by better capturing G × E interactions in MET studies (Jarquín 2017; Scott et al. 2021; Westhues et al. 2021; Montesinos-López et al. 2022).

The small n size and low haplotype diversity of the dataset (500 lines) is another area for future expansion. The Multi-parent Advanced Generation Inter Cross (MAGIC) wheat dataset (Scott et al. 2021) offered broad allelic diversity but still could be improved by increasing haplotype

variation (van de Wouw et al. 2010; Fradgley et al. 2019; Scott et al. 2021). A larger population with higher haplotype diversity could further improve the reliability and performance of the evaluated models (Norman et al. 2018).

Another direction for exploration is to expand our hyperparameter grid to tune other important GBM hyperparameters including tree depth (interaction.depth) and regularization parameters like minimum node size and colsample rate (Westhues et al. 2021). Additionally, tuning stochastic subsampling rates of 40-60%, which have been shown to improve performance, are efforts suggested in the founding literature (Friedman 2002). We suggest larger ranges and types of hyperparameter would be useful to find global optima of parameters for a more complete model optimization.

Future studies could address the stability of feature contributions or the performance trade-offs when optimizing model structural stability. One study identified a trade-off showing a ~2% reduction in predictive power for a 30% gain in structural stability (Bertsimas et al. 2025). Their work examined structural stability during model retraining, while our study focused on output stability across iterations. Applying a mixed integer optimization approach, which constrains variation in model structure, such as split variables and leaf values across successive retraining, could show whether the loci driving predictions across separate model training remain consistent, support feature selection efforts and provide evidence of predictive performance tradeoffs when structural stability is improved (Bertsimas et al. 2025).

While the performance gains from a low learning rate are substantially improved by boosting rounds, the computational demands from high boosting rounds can be improved, especially in time-sensitive applications. An effective model strategy to optimize computational costs is to utilize early stopping, allowing the model to find parameters that generalize well and mitigate excessive epochs that can degrade generalizability (Prechelt 2012). The gbm.fit function lacks early stopping; however, alternative gradient boosting packages, XGBoost and LightGBM, contain an early_stopping_rounds argument that can be directly used to set the number of boosting iterations the model can perform without improvement on a specified evaluation metric, after which the training automatically stops (Chen et al. 2014; Ke et al. 2017; lightgbm package - RDocumentation).

This study focussed on one modeling approach (GBM). In future work, benchmarking different algorithms (GBM vs. random forests vs. GBLUP, etc.) using the same multi-objective evaluation under the same cross-year prediction scenario would be useful for model selection, with each algorithm being individually optimized.

Our study demonstrates that model stability can be significantly improved without a necessary trade-off in performance. These findings highlight the utility and need for multi-objective optimization in genomic prediction, where stability is evaluated alongside predictive performance metrics. This work provides a reliable framework for tuning stochastic models to deliver reliable and consistent predictions required for use in breeding programs.

Data Availability

File S1 contains, Packages and Functions, Formulae of metrics and models, Hyperparameter Grid, Computing Environment.
File S2 contains, evaluation metric descriptive statistics used in data visualization.
File S3 contains, pairwise comparisons of the estimated marginal means and ANOVA tables
File S4 contains the complete evaluation metric results for each model configuration (stability metric per subset, performance metrics per iteration and subset)
File S5 contains the summary statistics for each trait-metric combination (aggregated across configurations)

The R scripts and datasets used for modelling, statistical analysis, and figure generation are available in the GitHub repository (https://github.com/HenryOmix/Multi-objective-Evaluation-and-Optimization-of-Stochastic-Gradient-Boosting-Machine). The specific version of the code used to produce the results in this manuscript is permanently archived on Zenodo:
HenryOmix. (2025).
HenryOmix/Multi-objective-Evaluation-and-Optimization-of-Stochastic-Gradient-Boosting-Machine: v.1.0.2 (v.1.0.2). Zenodo. https://doi.org/10.5281/zenodo.16266155

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Conflict of Interest

We declare that there are no conflicts of interest.

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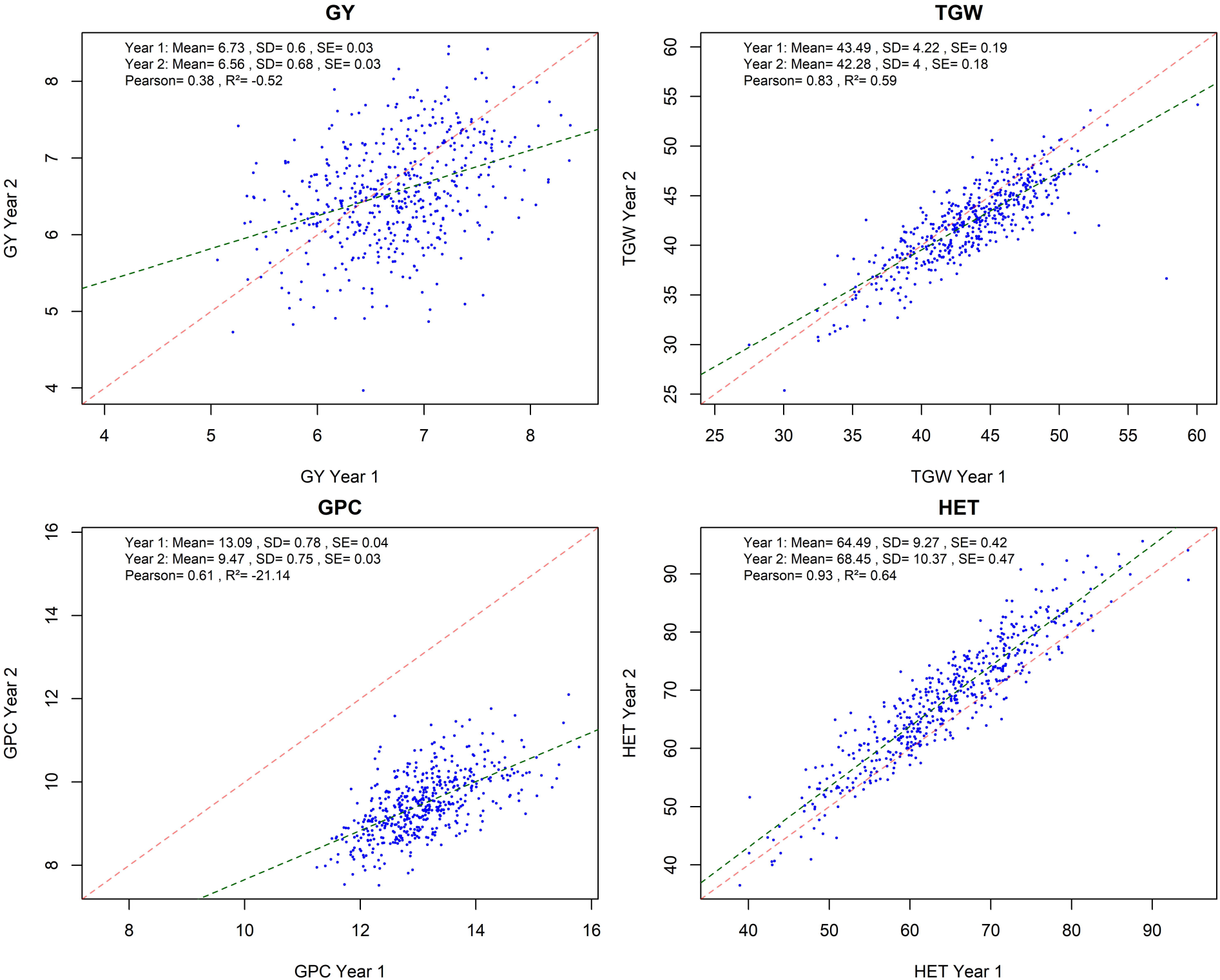
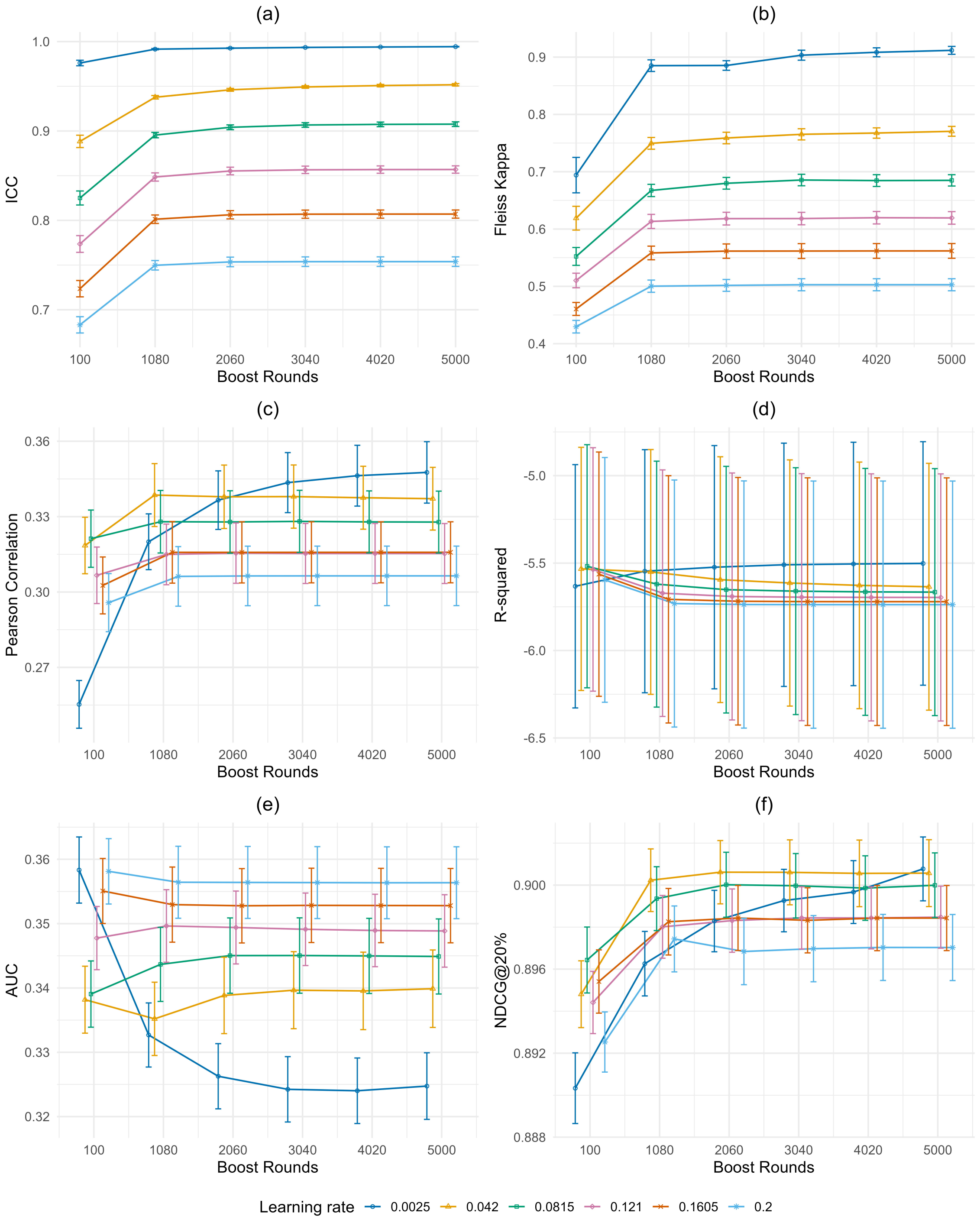
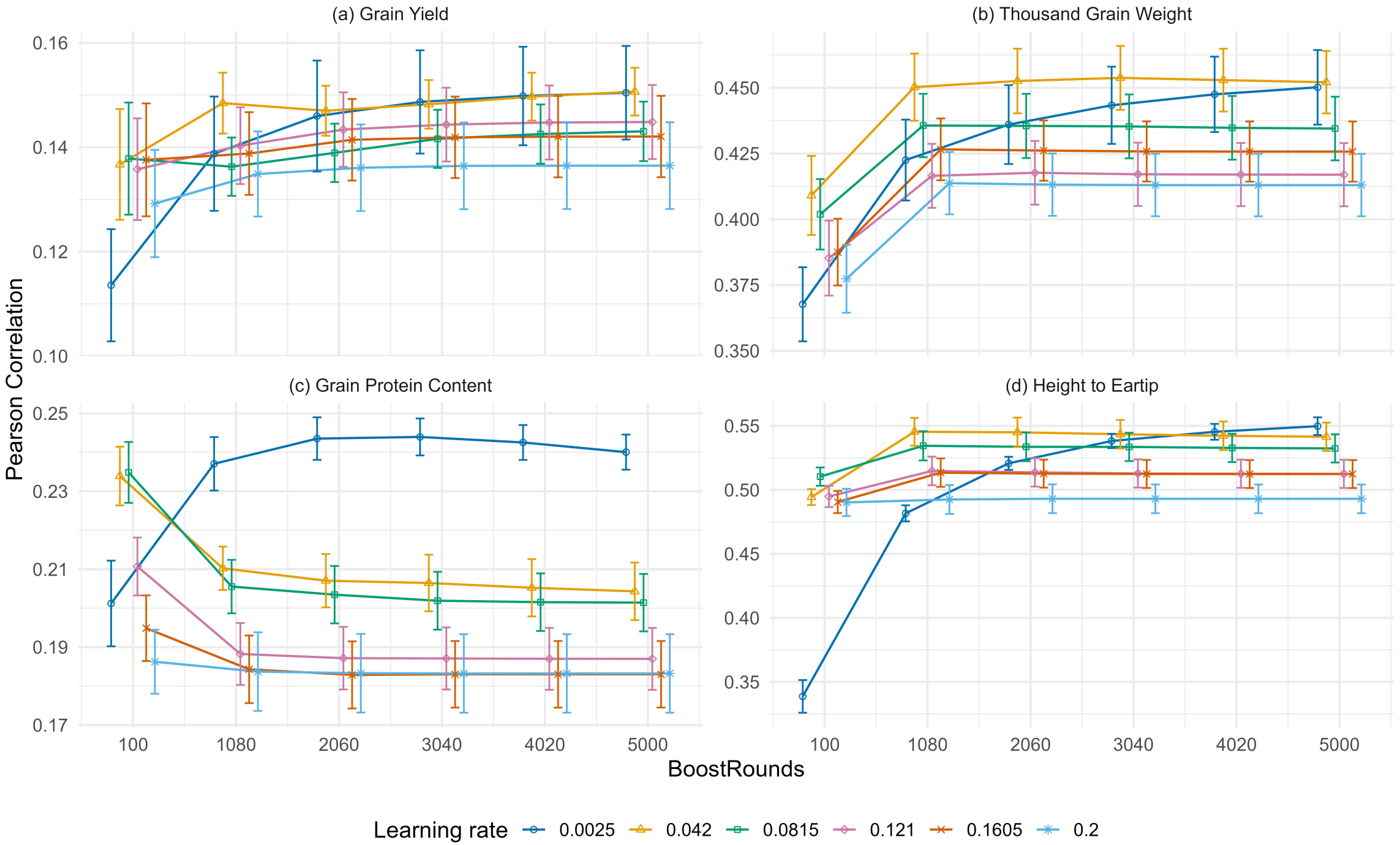
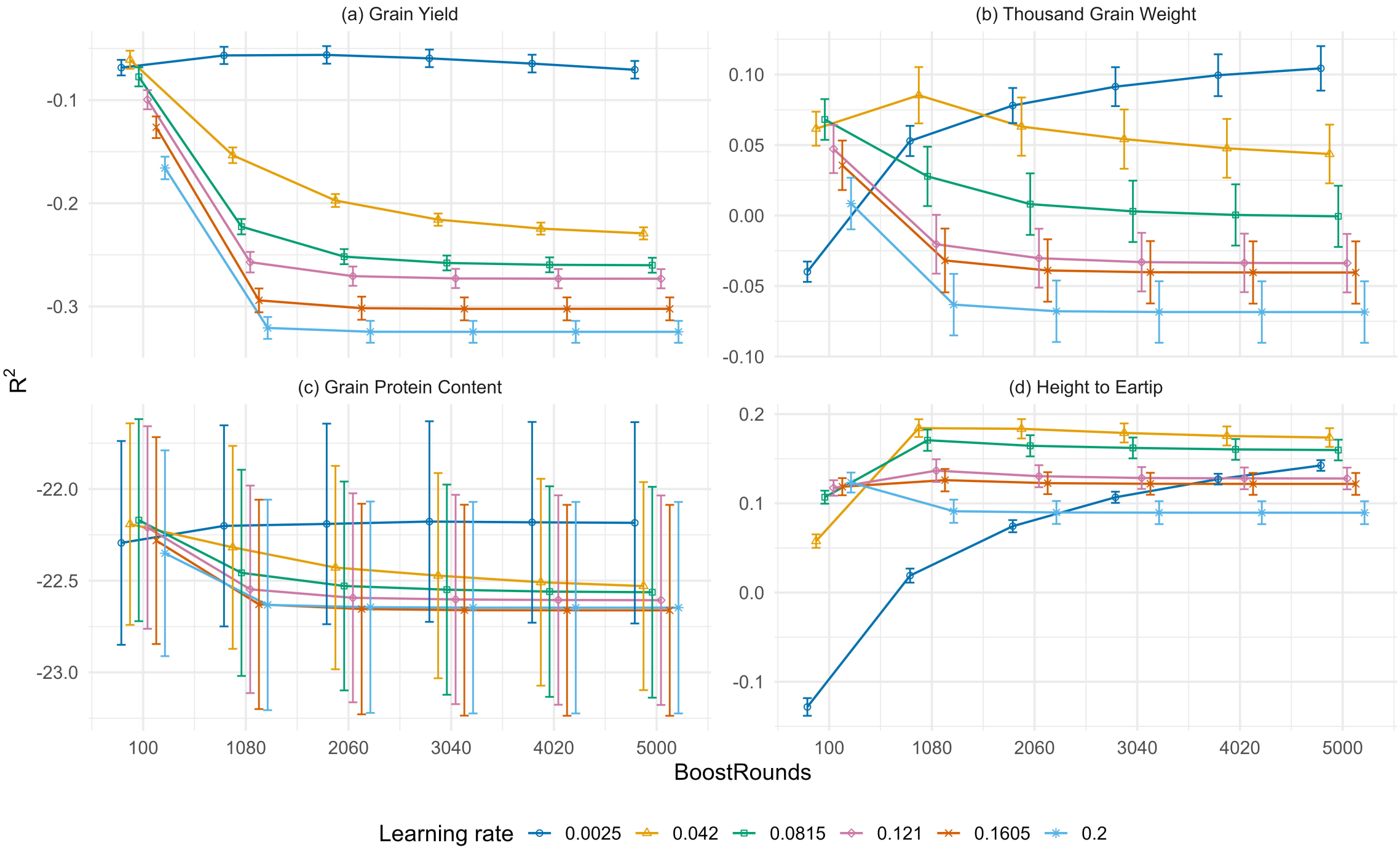
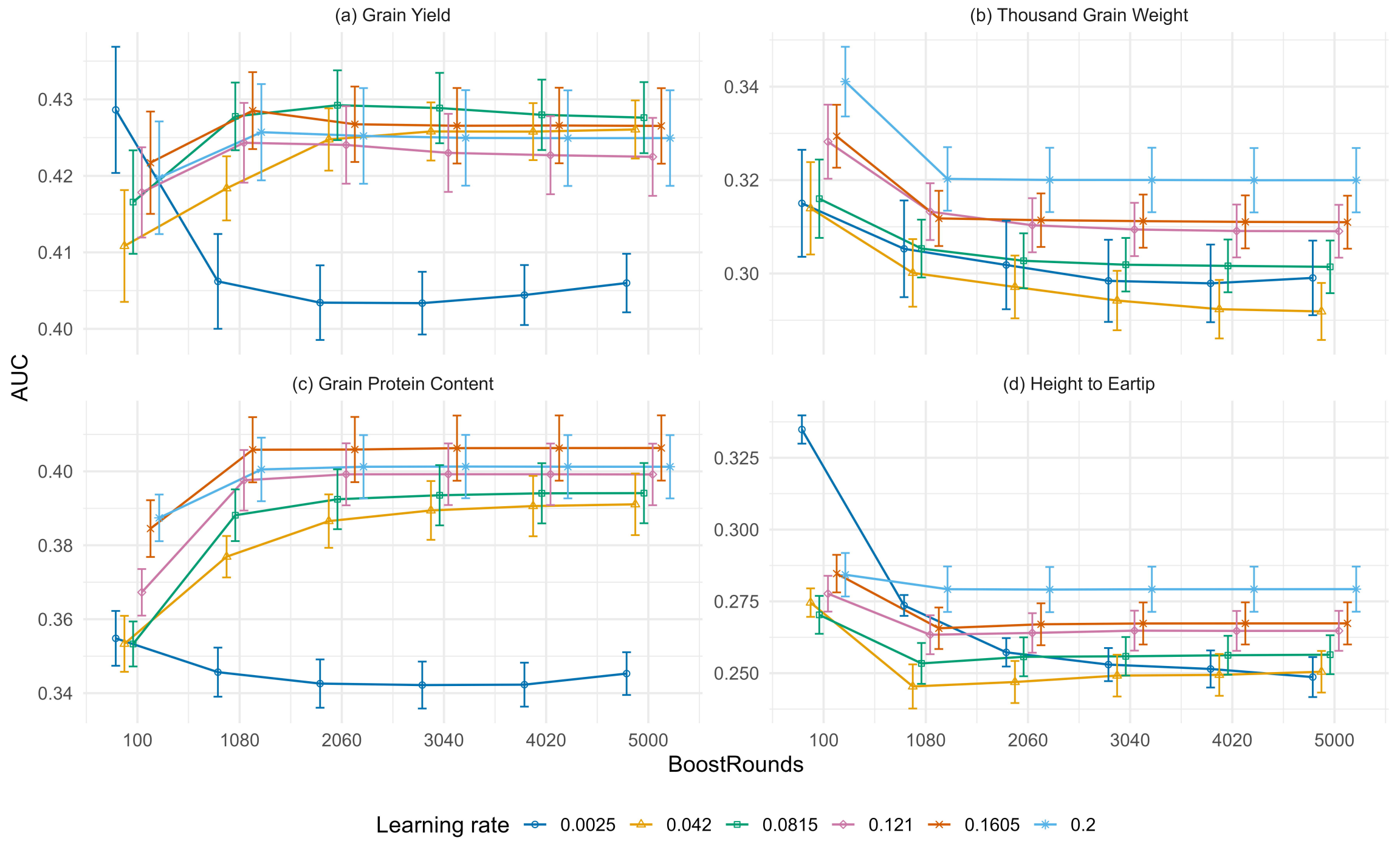
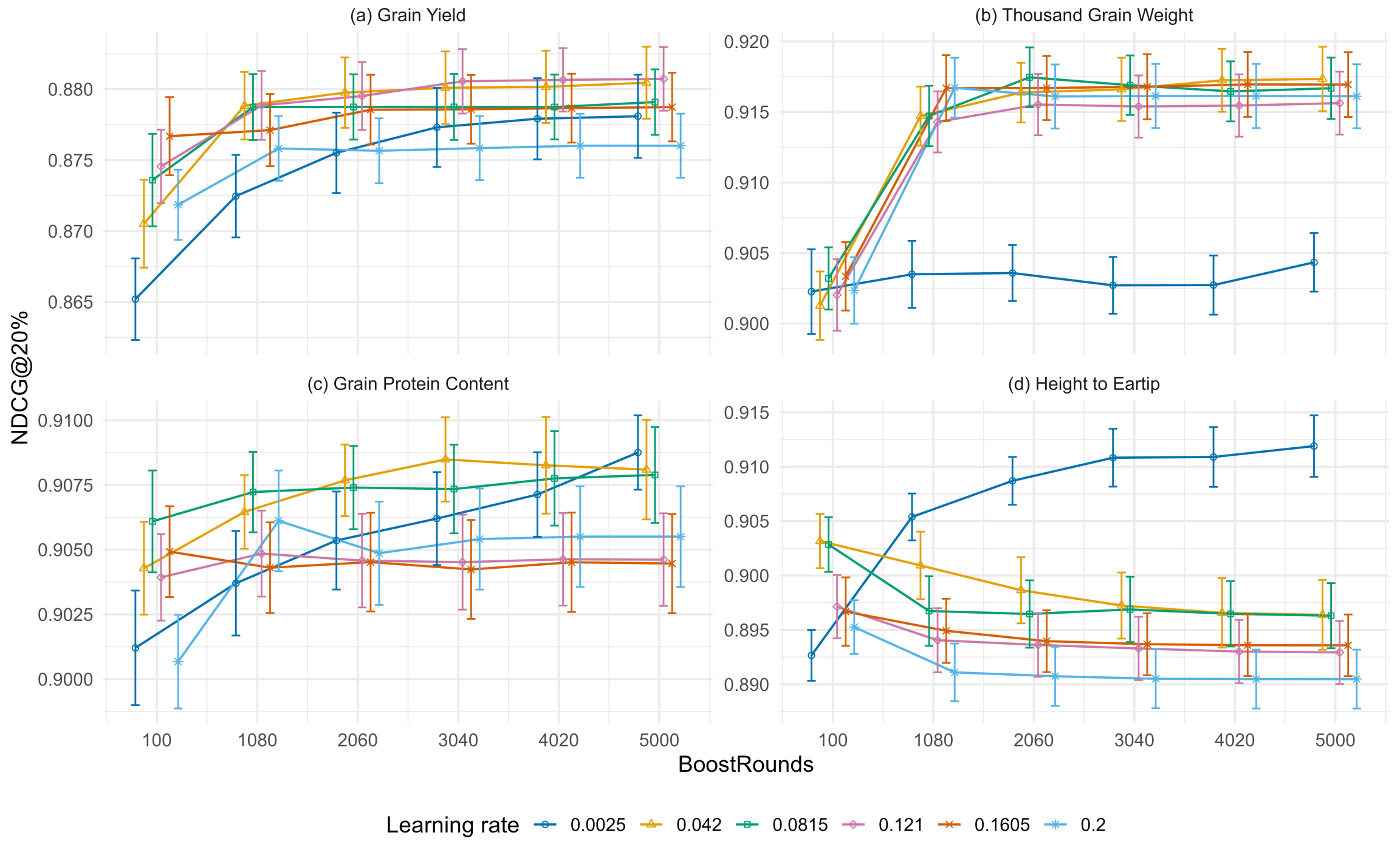

GY
Year 1: Mean= 6.73 , SD= 0.6 , SE= 0.03
Year 2: Mean= 6.56 , SD= 0.68 , SE= 0.03
Pearson= 0.38 , R²= -0.52
GY Year 2
GY Year 1
TGW
Year 1: Mean= 43.49 , SD= 4.22 , SE= 0.19
Year 2: Mean= 42.28 , SD= 4 , SE= 0.18
Pearson= 0.83 , R²= 0.59
TGW Year 2
TGW Year 1
GPC
Year 1: Mean= 13.09 , SD= 0.78 , SE= 0.04
Year 2: Mean= 9.47 , SD= 0.75 , SE= 0.03
Pearson= 0.61 , R²= -21.14
GPC Year 2
GPC Year 1
HET
Year 1: Mean= 64.49 , SD= 9.27 , SE= 0.42
Year 2: Mean= 68.45 , SD= 10.37 , SE= 0.47
Pearson= 0.93 , R²= 0.64
HET Year 2
HET Year 1

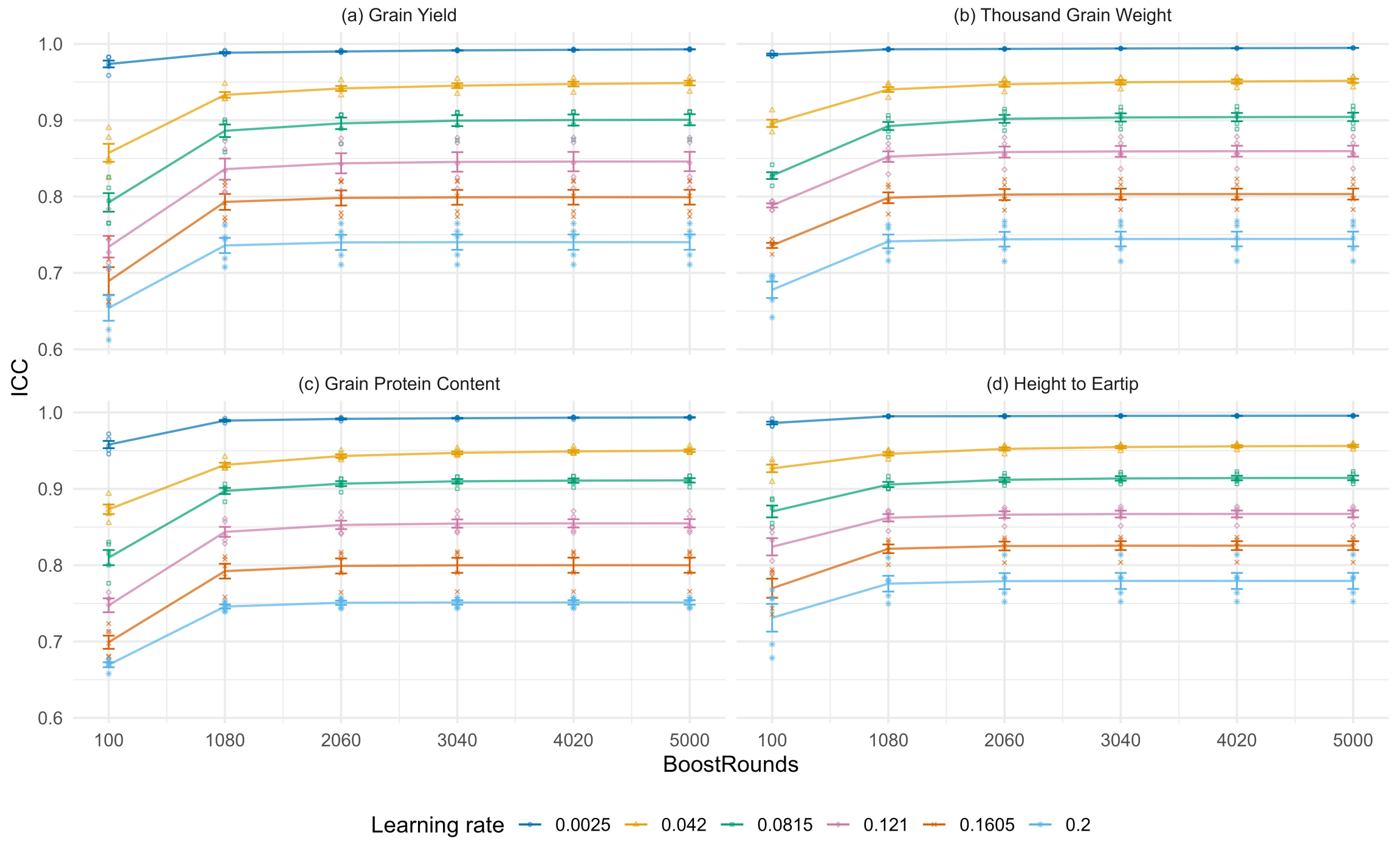

(a)
ICC
1.0
0.9
0.8
0.7
100
1080
2060
3040
4020
5000
Boost Rounds
(b)
Fleiss Kappa
0.9
0.8
0.7
0.6
0.5
0.4
100
1080
2060
3040
4020
5000
Boost Rounds
(c)
Pearson Correlation
0.36
0.33
0.30
0.27
100
1080
2060
3040
4020
5000
Boost Rounds
(d)
R-squared
-5.0
-5.5
-6.0
-6.5
100
1080
2060
3040
4020
5000
Boost Rounds
(e)
AUC
0.36
0.35
0.34
0.33
0.32
100
1080
2060
3040
4020
5000
Boost Rounds
(f)
NDCG@20%
0.900
0.896
0.892
0.888
100
1080
2060
3040
4020
5000
Boost Rounds
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2

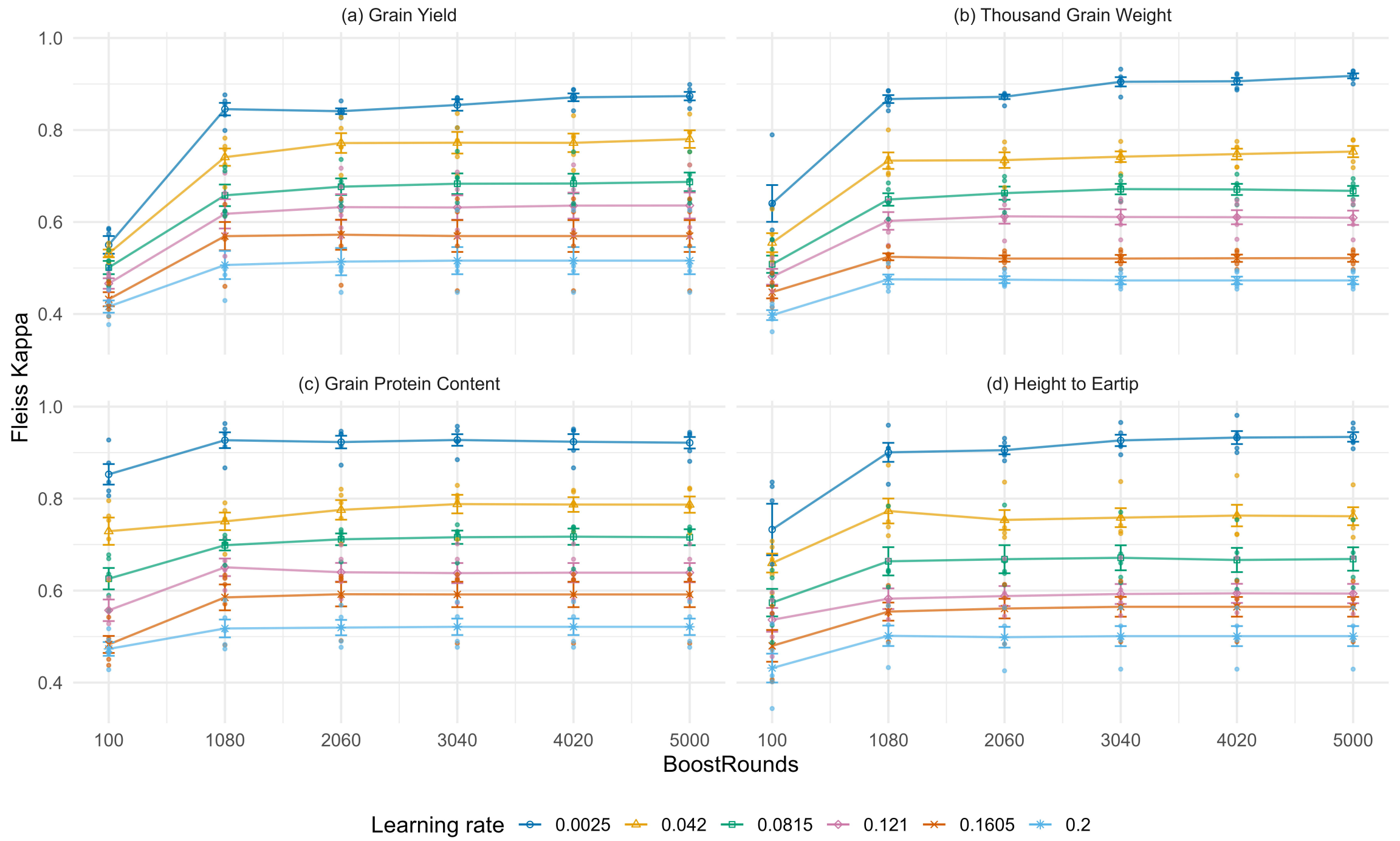

(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
Pearson Correlation
BoostRounds
0.16
0.14
0.12
0.10
0.450
0.425
0.400
0.375
0.350
0.25
0.23
0.21
0.19
0.17
0.55
0.50
0.45
0.40
0.35
100
1080
2060
3040
4020
5000
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2

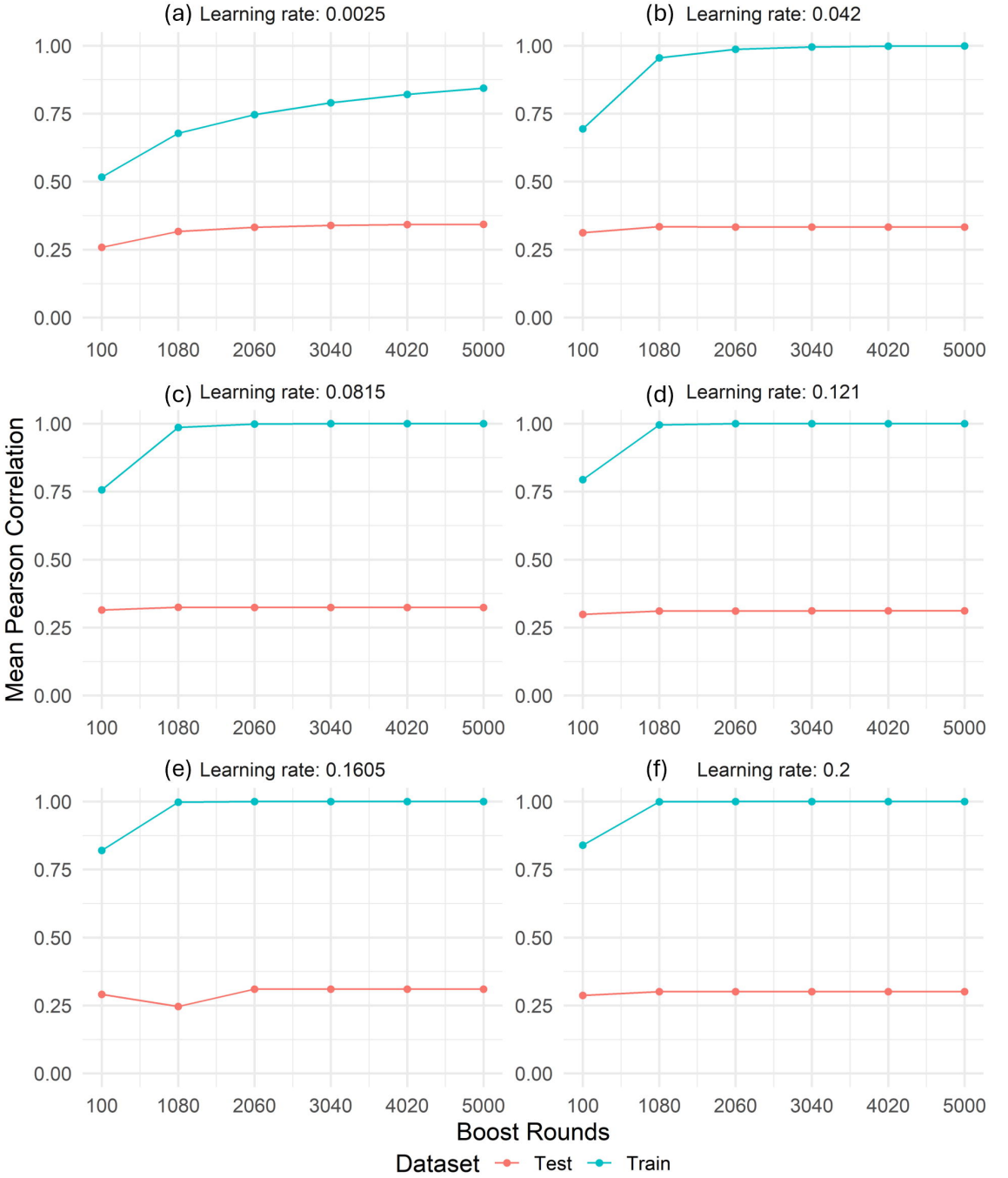

(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
R2
-0.1
-0.2
-0.3
0.10
0.05
0.00
-0.05
-0.10
-22.0
-22.5
-23.0
0.2
0.1
0.0
-0.1
100
1080
2060
3040
4020
5000
BoostRounds
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2


(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
AUC
0.43
0.42
0.41
0.40
0.34
0.32
0.30
0.40
0.38
0.36
0.34
0.325
0.300
0.275
0.250
100
1080
2060
3040
4020
5000
BoostRounds
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2


(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
NDCG@20%
BoostRounds
0.880
0.875
0.870
0.865
0.920
0.915
0.910
0.905
0.900
0.9100
0.9075
0.9050
0.9025
0.9000
0.915
0.910
0.905
0.900
0.895
0.890
100
1080
2060
3040
4020
5000
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2


(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
ICC
1.0
0.9
0.8
0.7
0.6
100
1080
2060
3040
4020
5000
BoostRounds
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2


(a) Grain Yield
(b) Thousand Grain Weight
(c) Grain Protein Content
(d) Height to Eartip
Fleiss Kappa
1.0
0.8
0.6
0.4
100
1080
2060
3040
4020
5000
BoostRounds
Learning rate
0.0025
0.042
0.0815
0.121
0.1605
0.2


(a) Learning rate: 0.0025
(b) Learning rate: 0.042
(c) Learning rate: 0.0815
(d) Learning rate: 0.121
(e) Learning rate: 0.1605
(f) Learning rate: 0.2
Mean Pearson Correlation
1.00
0.75
0.50
0.25
0.00
100
1080
2060
3040
4020
5000
Boost Rounds
Dataset
Test
Train