Supplementary Material 1- Calibration and Evaluation of Nwheat Simulation Model

2025-01-27

Introduction

This document contains the supplementary material for the manuscript titled **"Mitigating the Impact of Wheat Blast on Wheat Production in Bangladesh: A Study on Sowing Dates and Varietal Selection"**. It includes additional analyses, datasets, and code used to generate the results presented in the main text.

Packages

Importing data

The data was organized in the long format where each column is a variable and each observation is placed in a row. The code to import the data is:

```
## Load Data revised dataset (Received on September 21st, 2022)

dt<-gsheet2tbl("https://docs.google.com/spreadsheets/d/1USmV2yikAB1HYWVo8G65f8nEnKeYoEBR/edit?usp=sharin


# Display the first few rows of the dataset
head(dt)
```

```
## # A tibble: 6 x 33
##   Location year   REP   sowing variety  CHTD   EAD   GPD   GAD  GYAM  HIAM  GWGD
##   <chr>    <chr>  <chr>  <dbl> <chr>   <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 Dinajpur 2017-~ I          1 BARI G~     1   260    53 13806  4890    44    47
## 2 Dinajpur 2017-~ I          1 BARI G~     1   323    45 14600  4831    46    47
## 3 Dinajpur 2017-~ I          1 BARI G~     1   337    45 15030  4649    40    47
## 4 Dinajpur 2017-~ I          1 BARI G~     1   331    45 14994  4066    30    50
## 5 Dinajpur 2017-~ I          1 BARI G~     1   352    40 14080  4926    49    46
## 6 Dinajpur 2017-~ I          1 BARI G~     1   275    49 13475  5069    43    47
## # i 21 more variables: EDAP <dbl>, ADAP <dbl>, MDAP <dbl>, CWAA <dbl>,
## #   CWAM <dbl>, WB <dbl>, Lodging <dbl>, edapTmax <dbl>, edapTmin <dbl>,
## #   edapTmean <dbl>, edapRHmax <dbl>, edapRHmin <dbl>, edapRHmean <dbl>,
## #   mdapTmax <dbl>, mdapTmin <dbl>, mdapTmean <dbl>, mdapRHmax <dbl>,
## #   mdapRHmin <dbl>, mdapRHmean <dbl>, edapRain <dbl>, mdapRain <dbl>
```

```
# Summary of the dataset
summary(dt)
```

```
##    Location             year               REP                sowing  
##  Length:1485        Length:1485        Length:1485        Min.   :1  
##  Class :character   Class :character   Class :character   1st Qu.:2  
##  Mode  :character   Mode  :character   Mode  :character   Median :3  
##                                                           Mean   :3  
##                                                           3rd Qu.:4  
##                                                           Max.   :5  
##                                                                       
##    variety               CHTD         EAD            GPD       
##  Length:1485        Min.   :1    Min.   :190.0   Min.   :21.00  
##  Class :character   1st Qu.:1    1st Qu.:274.0   1st Qu.:40.00  
##  Mode  :character   Median :1    Median :301.0   Median :43.00  
##                     Mean   :1    Mean   :301.9   Mean   :43.39  
##                     3rd Qu.:1    3rd Qu.:327.0   3rd Qu.:46.00  
##                     Max.   :1    Max.   :498.0   Max.   :65.00  
##                     NA's   :21   NA's   :21      NA's   :105    
##       GAD             GYAM           HIAM            GWGD            EDAP      
##  Min.   : 6655   Min.   : 445   Min.   : 8.00   Min.   :11.00   Min.   :4.000  
##  1st Qu.:11211   1st Qu.:2600   1st Qu.:28.00   1st Qu.:36.00   1st Qu.:5.000  
##  Median :12842   Median :3536   Median :35.00   Median :42.00   Median :6.000  
##  Mean   :13058   Mean   :3461   Mean   :33.25   Mean   :40.23   Mean   :5.941  
##  3rd Qu.:14720   3rd Qu.:4265   3rd Qu.:39.00   3rd Qu.:46.00   3rd Qu.:7.000  
##  Max.   :23940   Max.   :6365   Max.   :53.00   Max.   :67.00   Max.   :9.000  
##  NA's   :105     NA's   :21     NA's   :105     NA's   :21      NA's   :21     
##       ADAP            MDAP            CWAA           CWAM      
##  Min.   :48.00   Min.   : 80.0   Min.   :1905   Min.   : 6000  
##  1st Qu.:63.00   1st Qu.: 97.0   1st Qu.:5621   1st Qu.: 9710  
##  Median :66.00   Median :101.0   Median :5828   Median :10368  
##  Mean   :65.38   Mean   :100.4   Mean   :5859   Mean   :10454  
##  3rd Qu.:69.00   3rd Qu.:105.0   3rd Qu.:6050   3rd Qu.:11150  
##  Max.   :85.00   Max.   :114.0   Max.   :9920   Max.   :18533  
##  NA's   :21      NA's   :21      NA's   :105    NA's   :105    
##        WB            Lodging          edapTmax        edapTmin    
##  Min.   : 0.000   Min.   : 0.000   Min.   :18.00   Min.   : 2.00  
##  1st Qu.: 0.000   1st Qu.: 0.000   1st Qu.:25.50   1st Qu.:10.00  
##  Median : 0.000   Median : 0.000   Median :26.90   Median :11.70  
##  Mean   : 8.016   Mean   : 3.685   Mean   :26.89   Mean   :11.58  
##  3rd Qu.: 0.000   3rd Qu.: 0.000   3rd Qu.:28.60   3rd Qu.:13.60  
##  Max.   :97.000   Max.   :90.000   Max.   :32.00   Max.   :19.00  
##  NA's   :21       NA's   :21       NA's   :105     NA's   :105    
##    edapTmean       edapRHmax        edapRHmin       edapRHmean   
##  Min.   :11.27   Min.   : 96.00   Min.   :16.20   Min.   :72.50  
##  1st Qu.:16.35   1st Qu.: 97.00   1st Qu.:32.75   1st Qu.:77.57  
##  Median :18.05   Median : 98.33   Median :38.00   Median :80.19  
##  Mean   :18.15   Mean   : 98.46   Mean   :38.72   Mean   :80.87  
##  3rd Qu.:20.00   3rd Qu.:100.00   3rd Qu.:44.00   3rd Qu.:83.89  
##  Max.   :25.96   Max.   :100.00   Max.   :64.00   Max.   :90.22  
##  NA's   :105     NA's   :105      NA's   :105     NA's   :105    
##     mdapTmax       mdapTmin       mdapTmean       mdapRHmax     
##  Min.   :29.7   Min.   : 1.00   Min.   :17.90   Min.   : 96.00  
##  1st Qu.:33.7   1st Qu.:10.33   1st Qu.:21.94   1st Qu.: 98.00  
##  Median :35.4   Median :13.00   Median :23.87   Median : 98.00  
##  Mean   :35.2   Mean   :11.94   Mean   :23.62   Mean   : 98.37  
##  3rd Qu.:36.4   3rd Qu.:14.90   3rd Qu.:25.21   3rd Qu.: 99.00  
```

```
## Max.   :38.5   Max.   :21.00   Max.   :29.31   Max.   :100.00
## NA's   :105    NA's   :105     NA's   :105     NA's   :105
##   mdapRHmin       mdapRHmean       edapRain      mdapRain
## Min.   : 0.00   Min.   :64.02   Min.   :0     Min.   :6
## 1st Qu.:15.00   1st Qu.:68.95   1st Qu.:0     1st Qu.:6
## Median :18.00   Median :70.94   Median :0     Median :6
## Mean   :16.61   Mean   :71.09   Mean   :0     Mean   :6
## 3rd Qu.:21.00   3rd Qu.:72.71   3rd Qu.:0     3rd Qu.:6
## Max.   :30.00   Max.   :79.32   Max.   :0     Max.   :6
## NA's   :105     NA's   :105     NA's   :105   NA's   :105
```

```r
# Working directory
work_dir <- getwd()
```

Experiment details

The experiments aiming for calibration and evaluation of the DSSAT-Nwheat simulation model consisted of four varieties (Table 1). The experiments were fully irrigated to maintain optimum soil moisture near field capacity. The land of the experimental fields was plowed with a two-wheel tractor, and it was exposed to sunshine for seven days before the subsequent plowing. After that, the land was deep-plowed and cross-plowed to obtain good tilth, which allows for better crop yield. All weeds and stubble were removed from the experimental field. The soil was treated with Furadan 5G, which contains Carbofuran, at 8 kg ha-1 to protect the young plants from insect attack. Recommended levels of mineral fertilizers for the region were applied: 100-27-40-20-1 kg ha-1 of N (nitrogen)-P (phosphorus)-K (potassium)-S (sulphur)-B (boron). Two-thirds of N and a full amount of the other fertilizers were applied immediately after final land preparation. The remaining N fertilizer was applied before the first irrigation (17-21 days after sowing). Before sowing, seeds were treated with Provax-200 WP, a fungicide recommended for controlling soil-borne fungi at the seedling stage. Seeds were sown in line continuously at 120 kg ha-1 for all varieties except BARI Gom 33 (140 kg ha-1) at a depth of 4-5 cm by making specific narrow furrows with an iron rod. After sowing, seeds were covered with soil and slightly pressed by hand. Seeds were repeatedly sown according to treatment dates using a 20 cm row-to-row distance. Three irrigations were applied during the whole growth period, where first irrigation was applied at 17-21 DAS (at crown root initiation), Second and third irrigations were applied at booting (50-55 DAS) and grain-filling (70-75 DAS) stages. A 2.5 cm water flow was applied in a 6 m2 plot during the first, second, and third irrigation. The experiment was conducted in a split-plot design with three replications. Main plots were assigned with five Sowing dates (i.e., Nov. 25, Dec. 05, Dec. 15, Dec. 25, and January 04), and subplots were with four wheat varieties (BARI Gom 26, BARI Gom 30, BARI Gom 32, BARI Gom 33). Plot size was 3x2 m (6 m2 for each subplot) (3m long 10 rows) in all three locations and years.

Table 1: A brief description of the four varieties used in the experiments

Name_of_the_variety	Pedigree	Year_of_Release
Bari Gom 26	ICTAL123/3/RAWAL87//VEE/HD 2285BD(JO)9585-0JO-3JE-0JE-0JE-HRDI-RC5DI	2010
Bari Gom 30	BAW677(PASTOR/3/VEE#5//DOVE/BUC)/BijoyBD(JA)1365S-0DI-15DI-3DI-HR12R3DI	2014
Bari Gom 32	SHATABDI/GOURABBD(DI)1686S-0DI-1DI-0DI-0DI-3DI	2017
Bari Gom 33	KACHU/SOLALACMSS09Y00580S-099Y-38M-0WGY-4B-0Y	2017

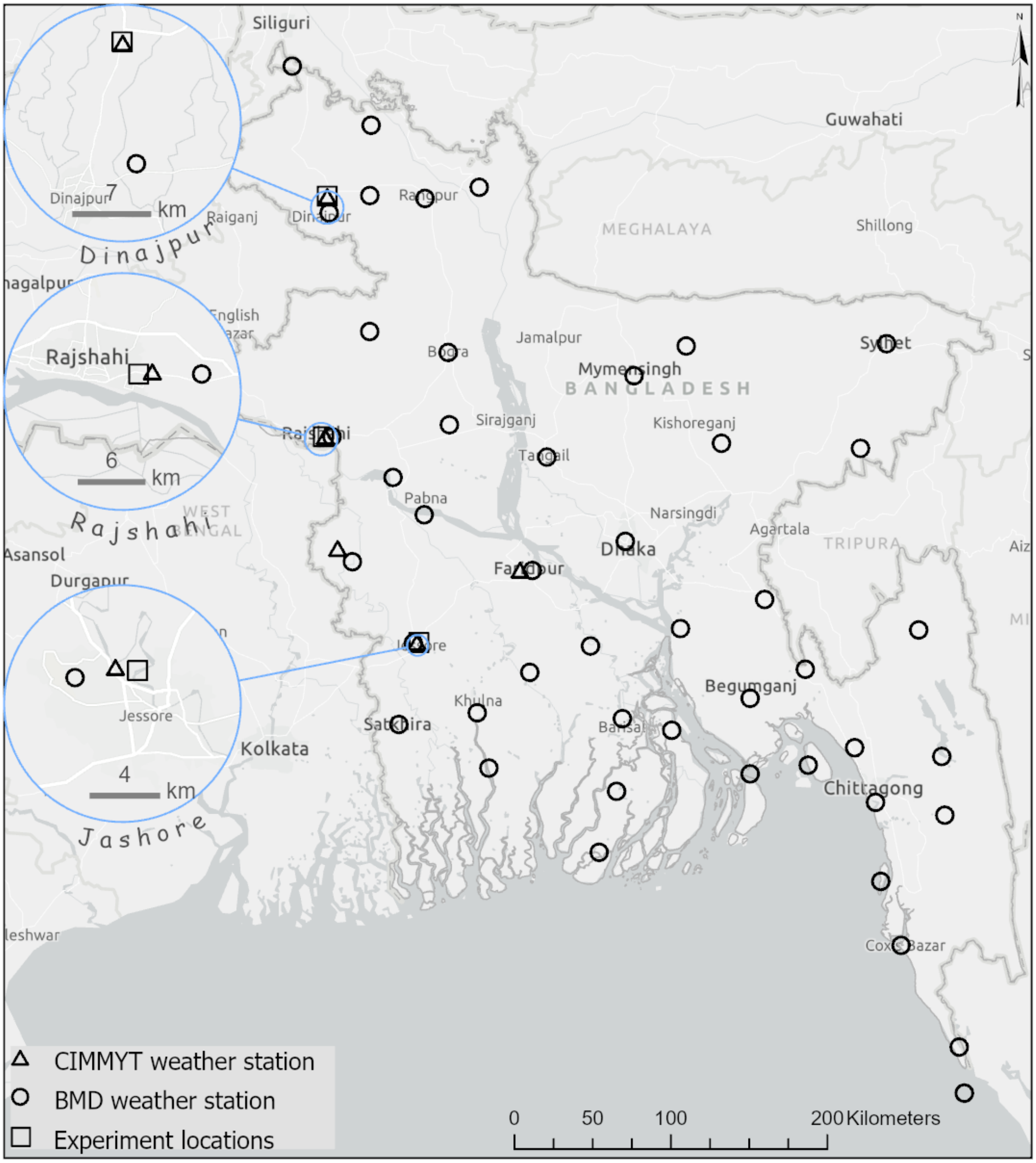


Figure 1: Map of Bangladesh highlighting the experiment locations (blue circles) and available automated weather stations.

Soil characteristics and weather data

Detailed soil characterization was conducted for each experimental location before planting. Soil excavations were dug in each site, and soil samples were taken from each layer. The collected samples were then analyzed for pH, Organic Carbon, Total Nitrogen, Phosphorus, exchangeable potassium (K), Sulfur, Calcium, Magnesium, Boro, Zinc, Iron, Manganese, Copper, Soil Moisture, Bulk Density, Hydraulic Conductivity, and Soil Texture. The Soil data tool (SBuild) present in DSSAT v. 4.8 was used to create the soil database, which was used for general simulation purposes. The data entered in this utility were the name of the country, name of the experimental site, site code, site coordinates, soil series, and classification. Measured soil characteristics taken from each profile were used to calculate the soil physical and chemical parameters needed to run the DSSAT- NWwheat model.

The observed weather variables used in this study include air temperature (C), relative humidity (%), and precipitation (mm) registered every 15 minutes. These weather variables were acquired from the Bangladesh Meteorological Department (BMD) and uploaded to a database. Solar radiation was retrieved from ERA5, a global atmospheric reanalysis dataset produced by the European Centre for Medium-Range Weather Forecasts (ECMWF).

Crop measurements

The evaluation of crop development was done by observing the phenology of the different wheat varieties and recording the time (days) it takes to attain each phenological phase. The recorded measurements were the grain number per plant, grain yield at maturity, harvest index at maturity, grain unit dry weight, emergence day after planting, anthesis day after planting, maturity days after planting, canopy weight at anthesis and canopy weight at maturity. All data were recorded from 1 meter long in five tagged rows in every plot. Yield and yield components measurements were taken at harvest maturity.

Estimating genotype specific parameters (GSPs)

Model calibration and model evaluation were carried out using independent observed experimental datasets. The model was calibrated by regulating only cultivar parameters using in-season data samples from optimum treatments from four consecutive cropping seasons. Treatments showing unexpectedly lower yields due to lodging or unexplained reasons were not used either for calibration or evaluation. For model calibration, a Bayesian method, namely the Generalized Likelihood Uncertainty Estimation (GLUE), was used to estimate the GSPs of the DSSAT-Nwheat model for the wheat varieties BARI GOM 26, BARI GOM 30, BARI GOM 32, and BARI GOM 33. The program uses Monte Carlo sampling from prior distributions of the coefficients and the Gaussian likelihood function to estimate the best coefficients for a given crop variety. The DSSAT-Nwheat model has GSPs that define a wheat variety's growth and development characteristics, shown in Table 2. The GLUE determines the probability distribution between observed data and those estimated by the model. Coefficients whose values exhibit the best adjustment were copied to the DSSAT cultivar file (Ferreira et al., 2024). The GLUESelect tool in the DSSAT v.4.8 performed the cultivar calibrations (Li et al., 2018). Each year, two files were created for 20 treatments representing each combination of variety (4) and sowing dates (5). First, the experimental file contains detailed information on the experimental conditions, such as environmental characteristics, soil analysis, initial soil moisture and N conditions, seedbed preparation and planting distance, irrigation and water management, fertilization, agrochemical applications, and harvest. The second is the observed data file having information on grain number per plant, grain yield at maturity, harvest index at maturity, grain unit dry weight, emergence in days after planting, anthesis in days after planting, maturity in days after planting, canopy weight at anthesis, and canopy weight at maturity. Four years of observed data from Dinajpur, Bangladesh (from 2017 to 2020) with five different planting dates for each wheat cultivar were utilized to calibrate the varieties' coefficients, respectively. For each cultivar, more than 360,000 simulation runs were performed during the GSP estimation process to evaluate the crop phenology and growth parameters. These simulations were performed inside the HiPerGator, the University of Florida supercomputer, through a parallelized version of GLUE that distributes the workload equally across the available CPU cores and merges the outputs to compute the likelihood values and evaluate which weighted parameter set better represents the observed data. A total of 80 cores were allocated for calibrating the genetic-specific coefficients of each cultivar.

Goodness-of-ft and evaluation of predictions

Goodness-of-fit refers to how well a calibrated model matches the data used for calibration. Prediction accuracy, on the other hand, measures how effectively a calibrated model simulates outcomes in environments different from those in the calibration dataset. For both goodness-of-fit and out-of-sample prediction, we used three metrics to measure the agreements between simulated and observed values. The root mean squared error (RMSE) (Eq. 1), the d-statistic (Eq. 2), and a skill score (Eq. 3) referred to as model efficiency (E) (Wallach et al., 2021).

The Root Mean Squared Error (RMSE) is defined as:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

RMSE is a common metric used to evaluate the performance of a model. It is an absolute measure of fit, meaning it measures how close the predicted values are to the true values. The RMSE takes on the same unit of deviation, Predicted-Observed, and it is commonly used in both model calibration and evaluation processes (Loague and Green, 1991).

The Index of Agreement (d) is defined as:

$$d = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(|y_i - \bar{y}| + |\hat{y}_i - \bar{y}|)^2}$$

Model efficiency is a dimensionless measure, an E = 1 corresponds to a perfect match of modeled output with the observed data and E < 1 for any realistic simulation. EF < 0 if the model predictions are worse than simply using the observed mean replace the simulated value. To some extent, $E \geq 0$ is a critical condition to conclude "goodness of match'' between the simulated and the observed (Wilmont et al., 2012; Yang, et al., 2014).

The Model Efficiency (E) is defined as:

$$E = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

In equations above Pi and Oi are the ith the model predictions and the pairwise-matched observations that are judged to be reliable, respectively, and n is the number of measurements summed for all varieties and sowing dates.

Exploratory data analysis for grain yield

Here we create a plot using the `metan` package to observe the distribution of some selected variables from the five years dataset. Exploratory data analysis is a critical process for performing initial investigations to find important relationships in the data, cleaning the data, spotting anomalies, and checking assumptions through data visualization. For consistency, we maintained only the varieties that were present in all years.

Figure 2: Mean wheat yield (kg ha^{-}¹) for different sowing dates across years and varieties in Dinajpur, Bangladesh. The bars represent the mean yield, while the error bars indicate the standard deviation of the mean. The figure highlights the effect of sowing date and variety on yield performance over multiple growing seasons.

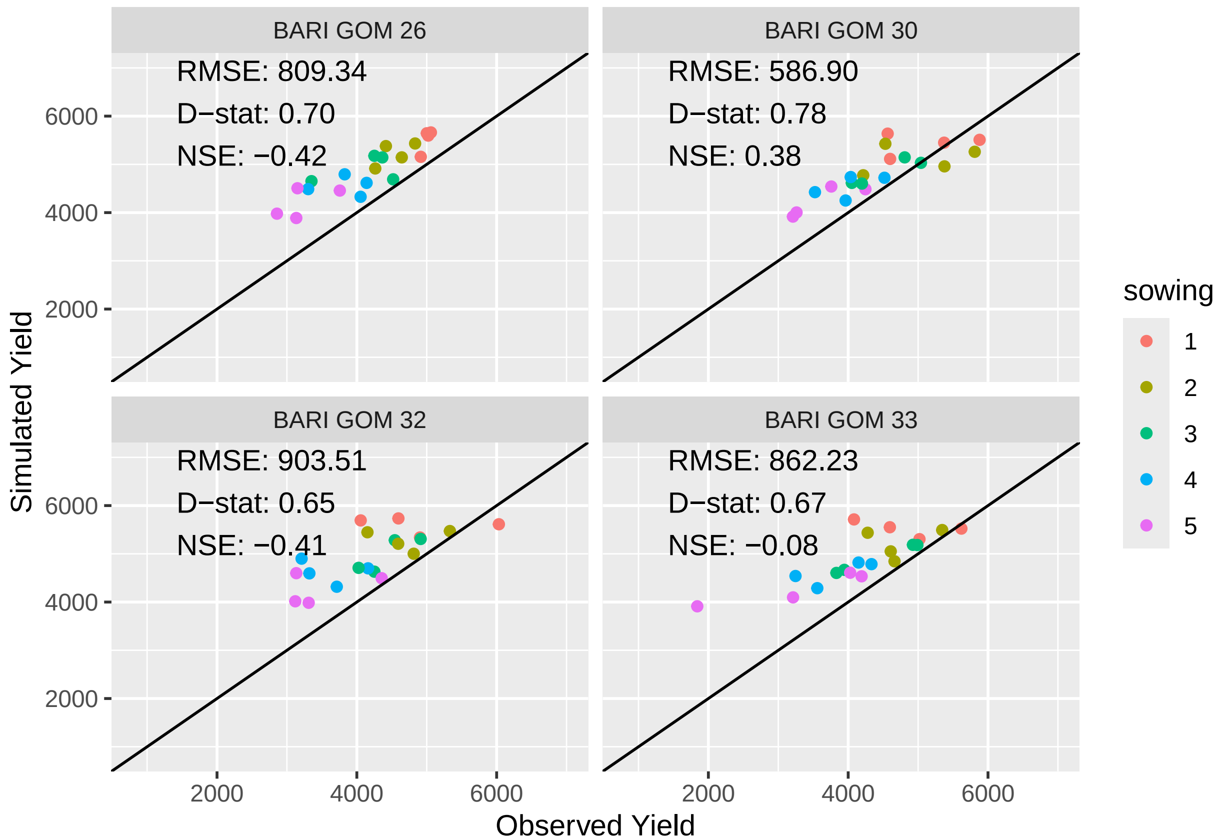
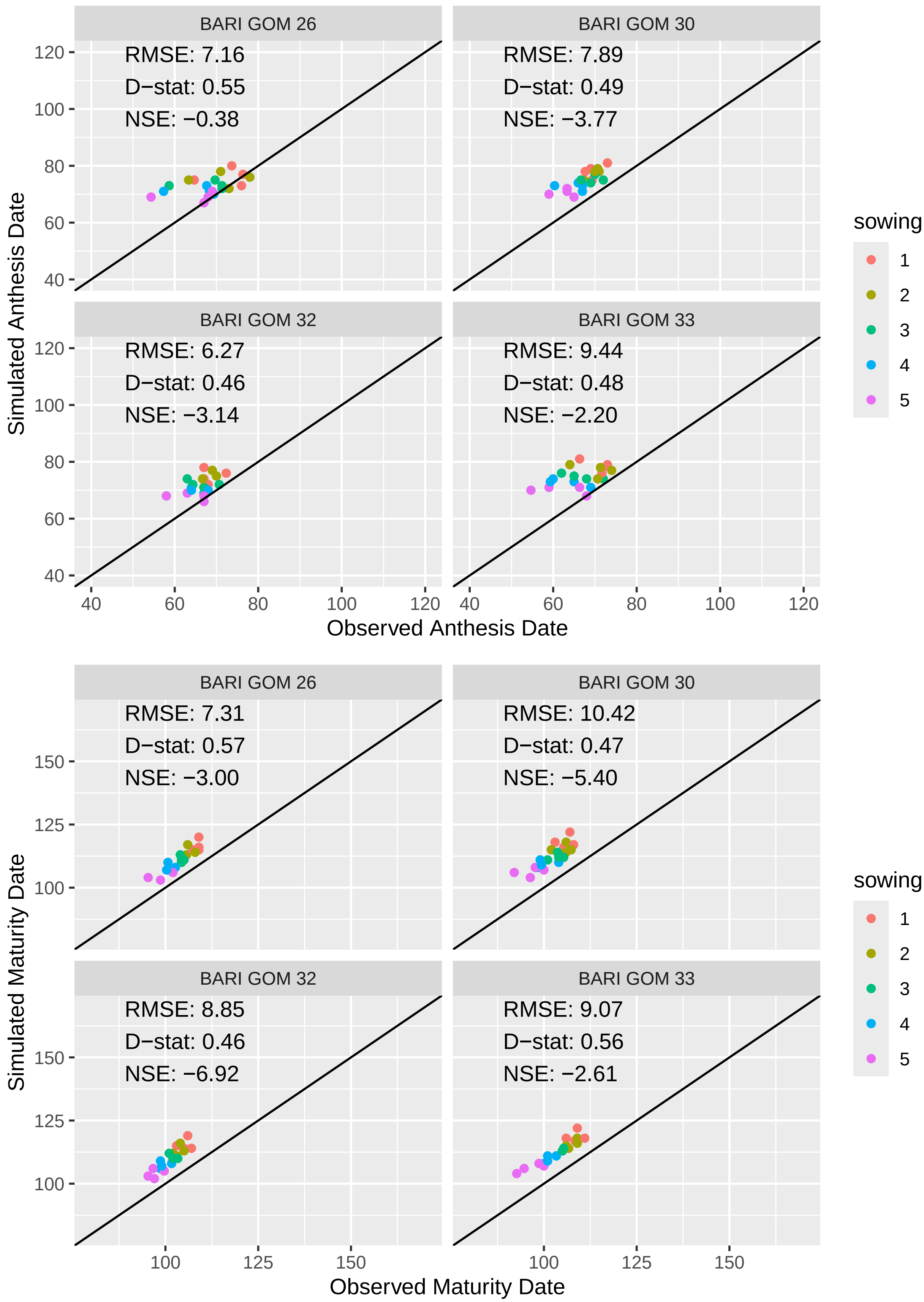


Figure 3: Identity plot comparing simulated grain yield (kg ha^{-}¹) against measured values.

Visualization



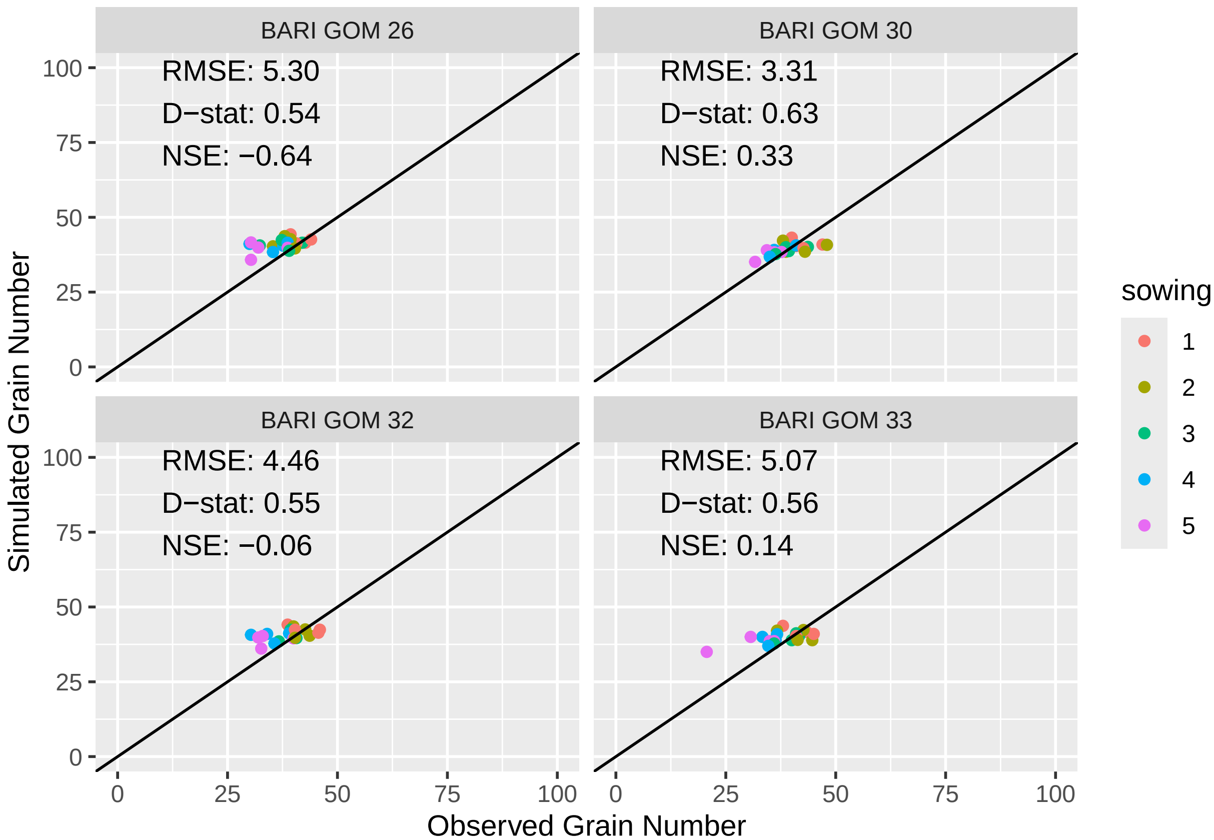


Figure 4: Identity plot comparing simulated harvest index against measured values.

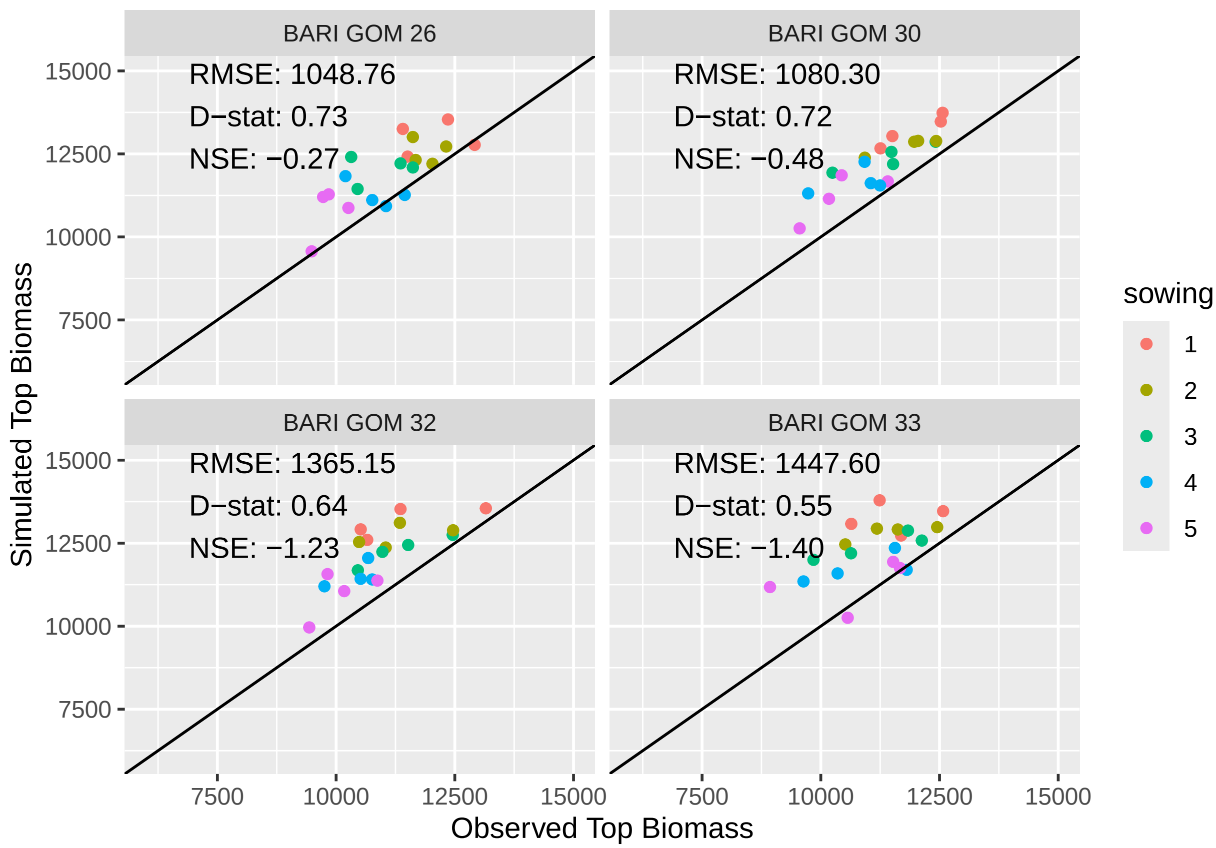


Figure 5: Identity plot comparing simulated biomass against measured values.

References

Ferreira, T. B., Shelia, V., Porter, C., Cadena, P. M., Cortasa, M. S., Khan, M. S., Pavan, W., & Hoogenboom, G. (2024). Enhancing crop model parameter estimation across computing environments: Utilizing the GLUE method and parallel computing for determining genetic coefficients. Computers and Electronics in Agriculture, 227, 109513. https://doi.org/10.1016/j.compag.2024.109513

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Wallach, D., Palosuo, T., Thorburn, P., Hochman, Z., Andrianasolo, F., Asseng, S., Basso, B., Buis, S., Crout, N., Dumont, B., Ferrise, R., Gaiser, T., Gayler, S., Hiremath, S., Hoek, S., Horan, H., Hoogenboom, G., Huang, M., Jabloun, M., … Seidel, S. J. (2021). Multi-model evaluation of phenology prediction for wheat in Australia. Agricultural and Forest Meteorology, 298–299, 108289. https://doi.org/10.1016/j.agrformet.2020.108289

Willmott, C. J., Robeson, S. M., & Matsuura, K. (2012). A refined index of model performance. International Journal of Climatology, 32(13), 2088–2094. https://doi.org/10.1002/joc.2419

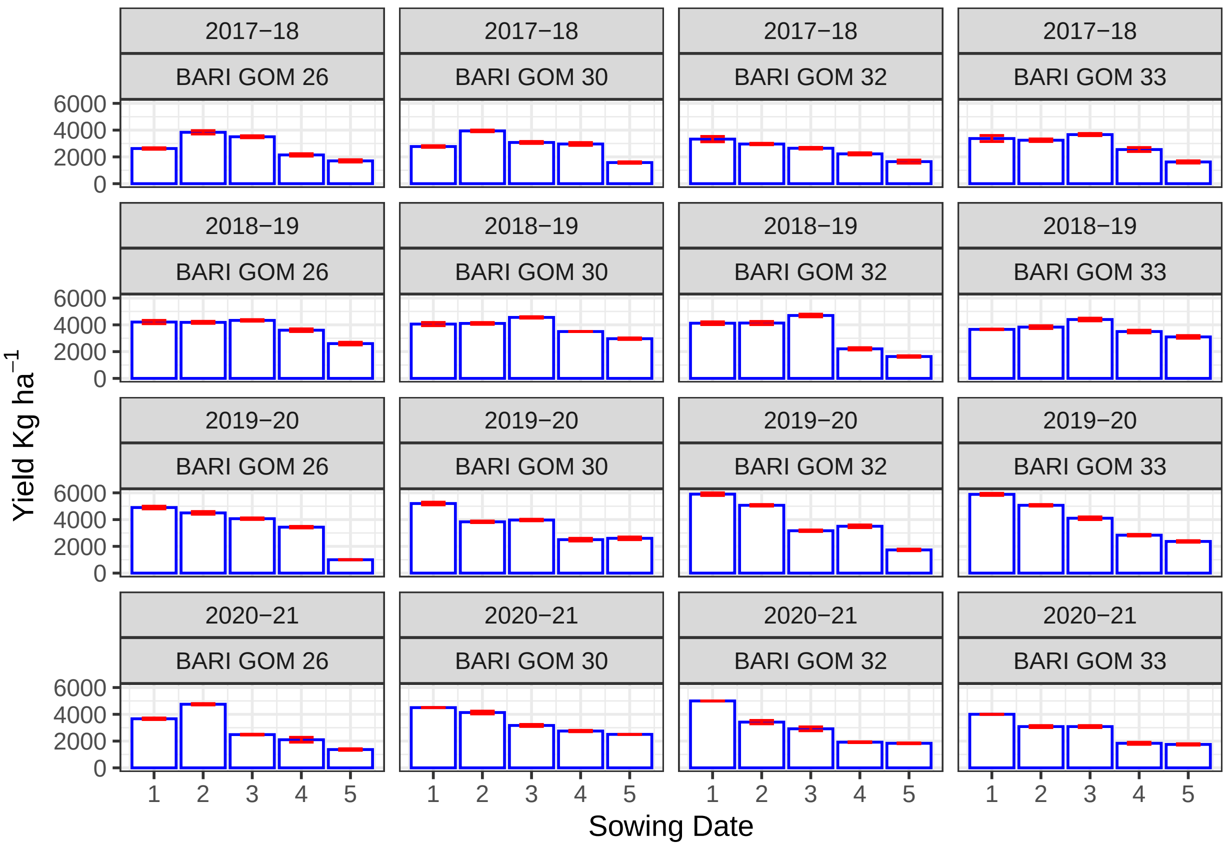

Figure 6: Mean wheat yield (kg ha^{-}¹) for different sowing dates across years and varieties in Rajshahi, Bangladesh. The bars represent the mean yield, while the error bars indicate the standard deviation of the mean. The figure highlights the effect of sowing date and variety on yield performance over multiple growing seasons.