Supplementary Materials

1. Stability Analysis of CPO-Based Hyperparameter Selection

This section provides supporting results for the internal validation experiment described in Section 2.5.2. The experiment evaluated the stability of the CPO-selected hyperparameters and examined whether the reported accuracy was overestimated due to information leakage. The multi-temporal configuration (CGI_{CR} + VIs) was selected as a representative case because it involves the largest number of input features among all examined setups and is therefore the most prone to overfitting.

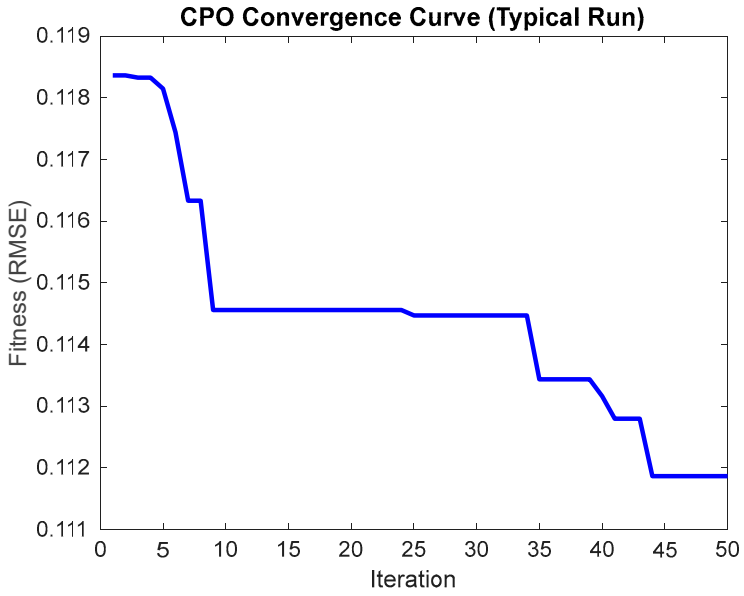

Figure S1. Convergence curve of CPO on the internal validation set (multi-temporal CGI_{CR} + VIs configuration). Fitness is defined as RMSE on the internal validation set (20% of the training data). The curve shown is from a representative run among 50 independent optimizations. Fitness drops sharply in the first 10 iterations and then flattens out, suggesting the optimizer converges efficiently.

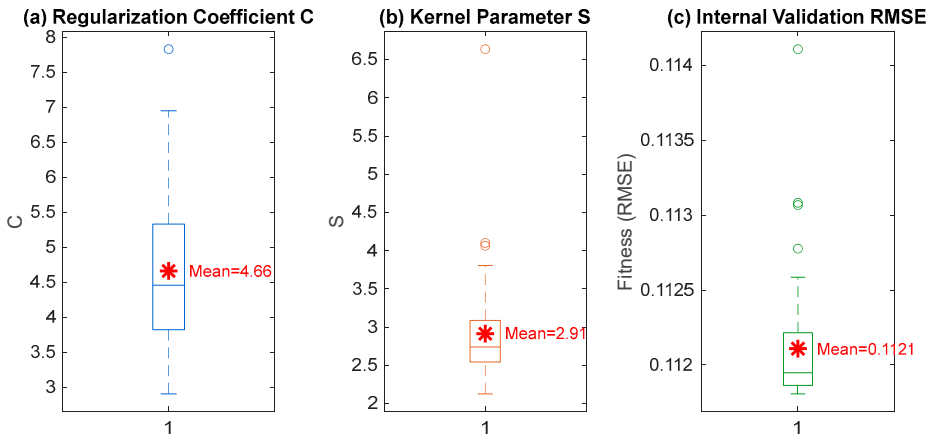

Figure S2. Distribution of CPO-selected hyperparameters over 50 independent runs. (a) Regularization coefficient C; (b) kernel parameter S; (c) internal validation RMSE (fitness). Red stars mark the mean values. The boxes are narrow and the standard deviations are small (C: 4.66 ± 1.12; S: 2.91 ± 0.70; Fitness: 0.1121 ± 0.0004), indicating that CPO consistently lands on similar solutions regardless of the random seed.

Table S1. Original vs. internal-validation CPO-KELM performance on the independent test set. "Original" = hyperparameters tuned on the full training set. "Internal validation" = hyperparameters selected by a stricter procedure: (i) redefining fitness on the internal validation set only; (ii) running CPO 50 times; (iii) picking the best parameters (C = 3.59, S = 2.69); (iv) retraining on the full training set, then testing. The two results are close ($\Delta R^2 \approx 0.031$), confirming that the reported accuracy is not artificially inflated by information leakage.

Model configuration	**Original CPO-KELM (R^2 / RMSE)**	**Internal validation CPO-KELM (R^2 / RMSE)**
Multi-temporal (CGICR+VIs)	0.920 / 515.7 kg/ha	0.889 / 555.9 kg/ha

Table S2. Growth-stage contribution analysis based on feature-group removal experiments.

Comparison	Full_Model	Reduced_Model	Full_R2	Reduced_R2	Delta_R2	Delta_R2_STD	Delta_R2_CI95	Full_RMSE	Reduced_RMSE	Delta_RMSE	Delta_RMSE_STD	Delta_RMSE_CI95	Delta_RPD	Delta_RPD_STD	Delta_RPD_CI95
ALL vs Remove J	ALL_FULL	ALL_REMOVE_J	0.82629	0.83397	-0.00768	0.013918145	0.002727956	621.11239	606.89828	-14.21411	23.45818294	4.597803857	-0.059891842	0.102332225	0.020057116
ALL vs Remove B	ALL_FULL	ALL_REMOVE_B	0.82629	0.83537	-0.00908	0.018276595	0.003582213	621.11239	601.846	-19.26639	33.68640118	6.602534631	-0.080062086	0.158472453	0.031060601
ALL vs Remove H	ALL_FULL	ALL_REMOVE_H	0.82629	0.81801	0.00828	0.014010155	0.00274599	621.11239	634.87959	13.7672	22.41938887	4.394200218	0.045899785	0.095504803	0.018718941
ALL vs Remove F	ALL_FULL	ALL_REMOVE_F	0.82629	0.7989	0.02739	0.021733415	0.004259749	621.11239	665.89641	44.78402	31.10649651	6.096873316	0.161320482	0.123481617	0.024202397
ALL vs ONLY J	ALL_FULL	ONLY_J	0.82629	0.70161	0.12468	0.071698144	0.014052836	621.11239	814.74392	193.63153	100.9720488	19.79052157	0.552782638	0.265046688	0.051949151
ALL vs ONLY B	ALL_FULL	ONLY_B	0.82629	0.70705	0.11924	0.055980357	0.01097215	621.11239	798.71561	177.60322	69.83739568	13.68812955	0.516974442	0.196211745	0.038457502
ALL vs ONLY H	ALL_FULL	ONLY_H	0.82629	0.82315	0.00314	0.026340436	0.005162726	621.11239	624.68206	3.56967	46.76815157	9.166557707	0.004678087	0.186978456	0.036647777
ALL vs ONLY F	ALL_FULL	ONLY_F	0.82629	0.83927	-0.01298	0.024412275	0.004784806	621.11239	592.13586	-28.97653	40.80598865	7.997973776	-0.127978798	0.175945438	0.034485306
ALL vs J+B	ALL_FULL	J+B	0.82629	0.73306	0.09323	0.048579177	0.009521519	621.11239	766.4443	145.33191	64.58228057	12.65812699	0.445201601	0.191883345	0.037609136
ALL vs H+F	ALL_FULL	H+F	0.82629	0.84746	-0.02117	0.02061629	0.004040793	621.11239	577.15939	-43.953	39.85861364	7.812288273	-0.199792611	0.189925813	0.037225459
ALL vs J+B+H	ALL_FULL	J+B+H	0.82629	0.7989	0.02739	0.021733415	0.004259749	621.11239	665.89641	44.78402	31.10649651	6.096873316	0.161320482	0.123481617	0.024202397
ALL vs B+H+F	ALL_FULL	B+H+F	0.82629	0.83397	-0.00768	0.013918145	0.002727956	621.11239	606.89828	-14.21411	23.45818294	4.597803857	-0.059891842	0.102332225	0.020057116
ALL vs VI	ALL_FULL	VI_FULL	0.82629	0.79571	0.03058	0.024951338	0.004890462	621.11239	673.83427	52.72188	35.88353716	7.033173283	0.18393186	0.128762654	0.02523748
ALL vs CGI	ALL_FULL	CGI_FULL	0.82629	0.75079	0.0755	0.053314675	0.010449676	621.11239	740.16074	119.04835	81.58905909	15.99145558	0.383145139	0.26471081	0.051883319
VI Remove J	VI_FULL	VI_REMOVE_J	0.79571	0.79964	-0.00393	0.019016874	0.003727307	673.83427	664.15999	-9.67428	28.00682961	5.489338603	-0.031516591	0.103854392	0.020355461
VI Remove B	VI_FULL	VI_REMOVE_B	0.79571	0.80423	-0.00852	0.014829318	0.002906546	673.83427	656.88896	-16.94531	29.27283397	5.737475459	-0.054622936	0.096357865	0.018886142
VI Remove H	VI_FULL	VI_REMOVE_H	0.79571	0.78684	0.00887	0.016645839	0.003262584	673.83427	686.73083	12.89656	23.31218197	4.569187665	0.039122465	0.079221993	0.015527511
VI Remove F	VI_FULL	VI_REMOVE_F	0.79571	0.78297	0.01274	0.021991559	0.004310346	673.83427	694.91687	21.0826	34.70438662	6.802059778	0.065672723	0.110988062	0.02175366
CGI Remove J	CGI_FULL	CGI_REMOVE_J	0.75079	0.72302	0.02777	0.041381413	0.008110757	740.16074	778.34979	38.18905	56.50595718	11.07516761	0.09461363	0.147935113	0.028995282
CGI Remove B	CGI_FULL	CGI_REMOVE_B	0.75079	0.76698	-0.01619	0.037039617	0.007259765	740.16074	714.806	-25.35474	49.82351737	9.765409404	-0.074400062	0.165957094	0.03252759
CGI Remove H	CGI_FULL	CGI_REMOVE_H	0.75079	0.7344	0.01639	0.044051599	0.008634113	740.16074	759.92023	19.75949	60.08316897	11.77630112	0.053170165	0.153412058	0.030068763
CGI Remove F	CGI_FULL	CGI_REMOVE_F	0.75079	0.615	0.13579	0.076487577	0.014991565	740.16074	923.09092	182.93018	87.28121396	17.10711794	0.384612995	0.177657256	0.034820822

Note: This table presents the full ablation results corresponding to Table 9 in the main text. All experiments were conducted using the full raw feature sets without VIF pre-filtering, to preserve complete stage-specific information for contribution assessment. $\Delta R^2 = R^2_{complete} - R^2_{reduced}$, $\Delta RMSE = RMSE_{reduced} - RMSE_{complete}$, and $\Delta RPD = RPD_{complete} - RPD_{reduced}$. Positive values indicate performance deterioration after removing the corresponding stage, whereas negative values indicate potential predictive redundancy or noise. Win rate represents the percentage of paired partitions in which the complete model outperformed the corresponding reduced model.