

Overall variable distributions by site

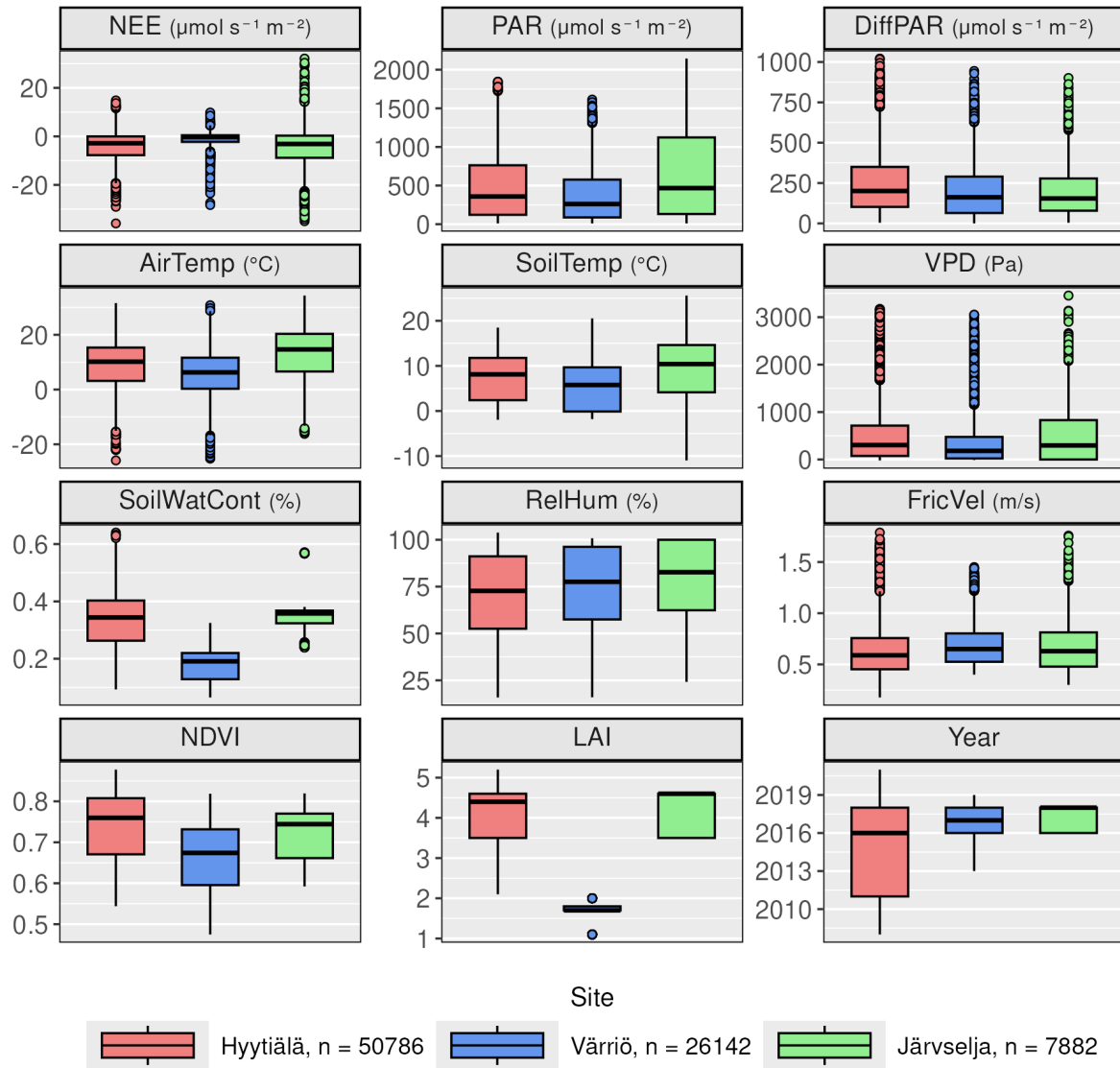


Figure A1: Boxplots showing the distribution of all input variables as well as NEE and the origin year across Värriö, Hyytiälä, and Järvelja.

Analysis of PAR and DiffPAR SHAP across model architectures

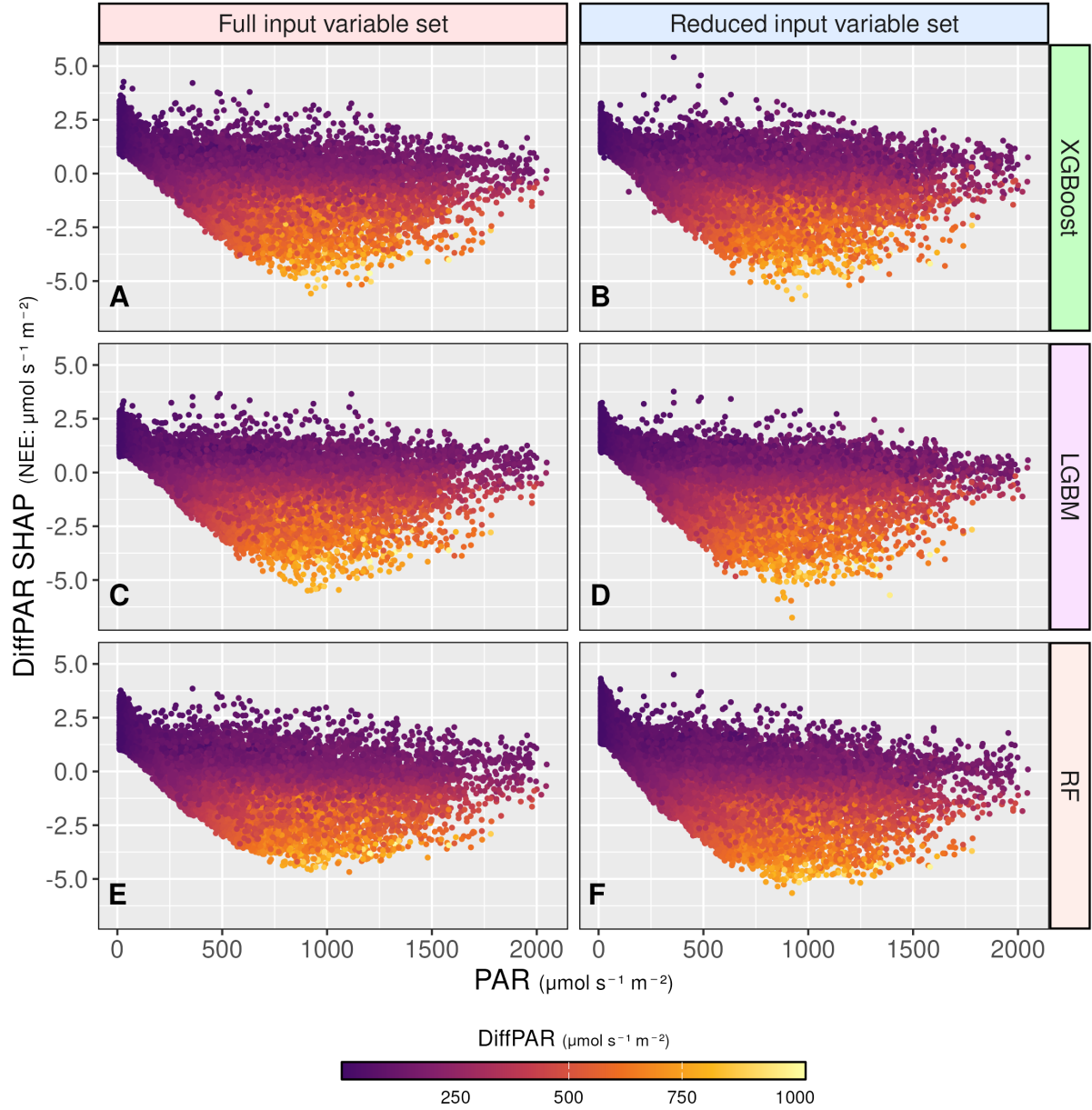


Figure A2: Scatterplots showing the relationship between PAR and DiffPAR SHAP across both input configurations, full and reduced, and all three ML models: XGBoost, Random Forest, and LGBM.

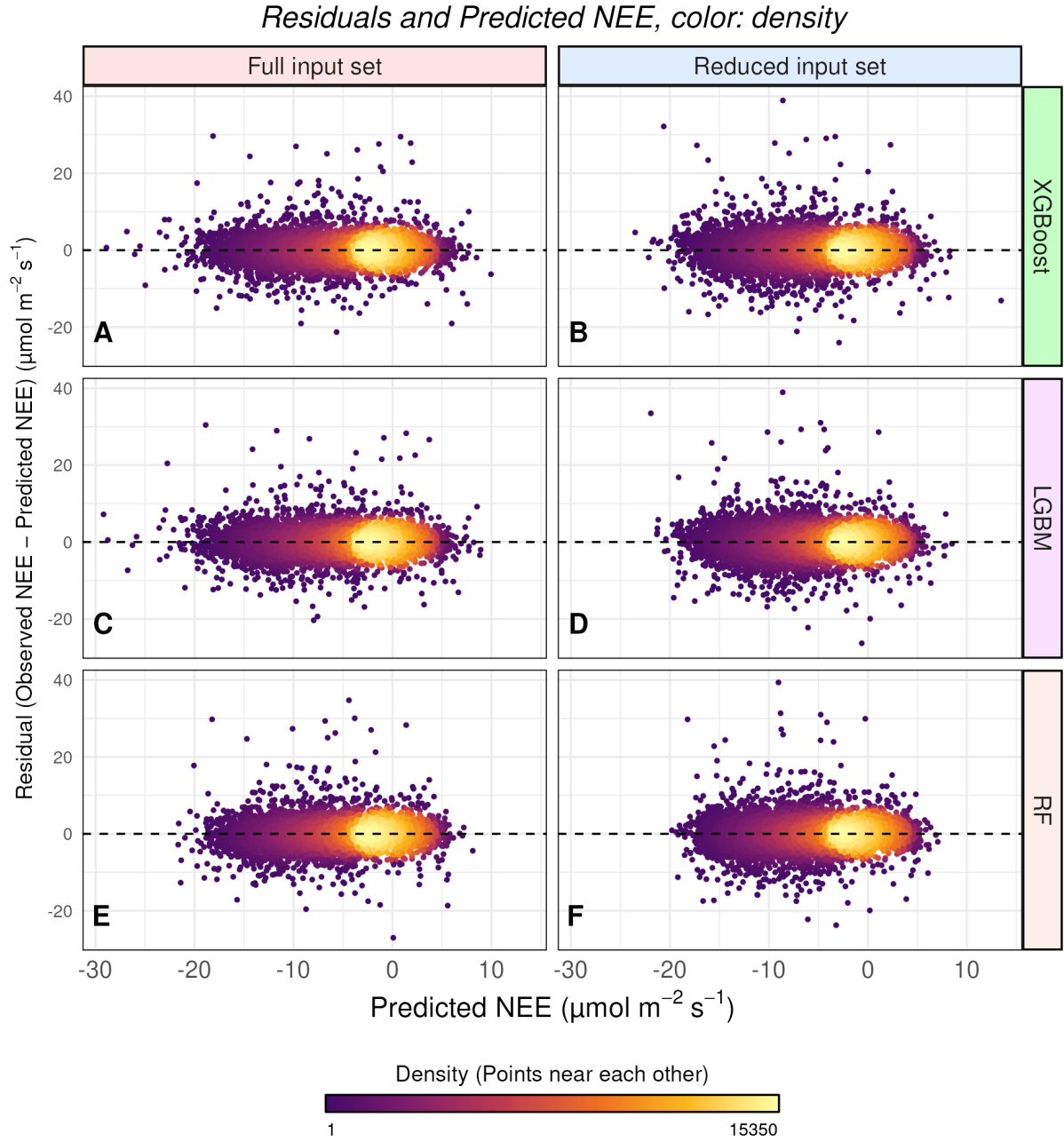


Figure A3: Residuals of the different ML models across both input configurations. A residual is the observed value minus the model-predicted value for a data point, i.e. the prediction error.

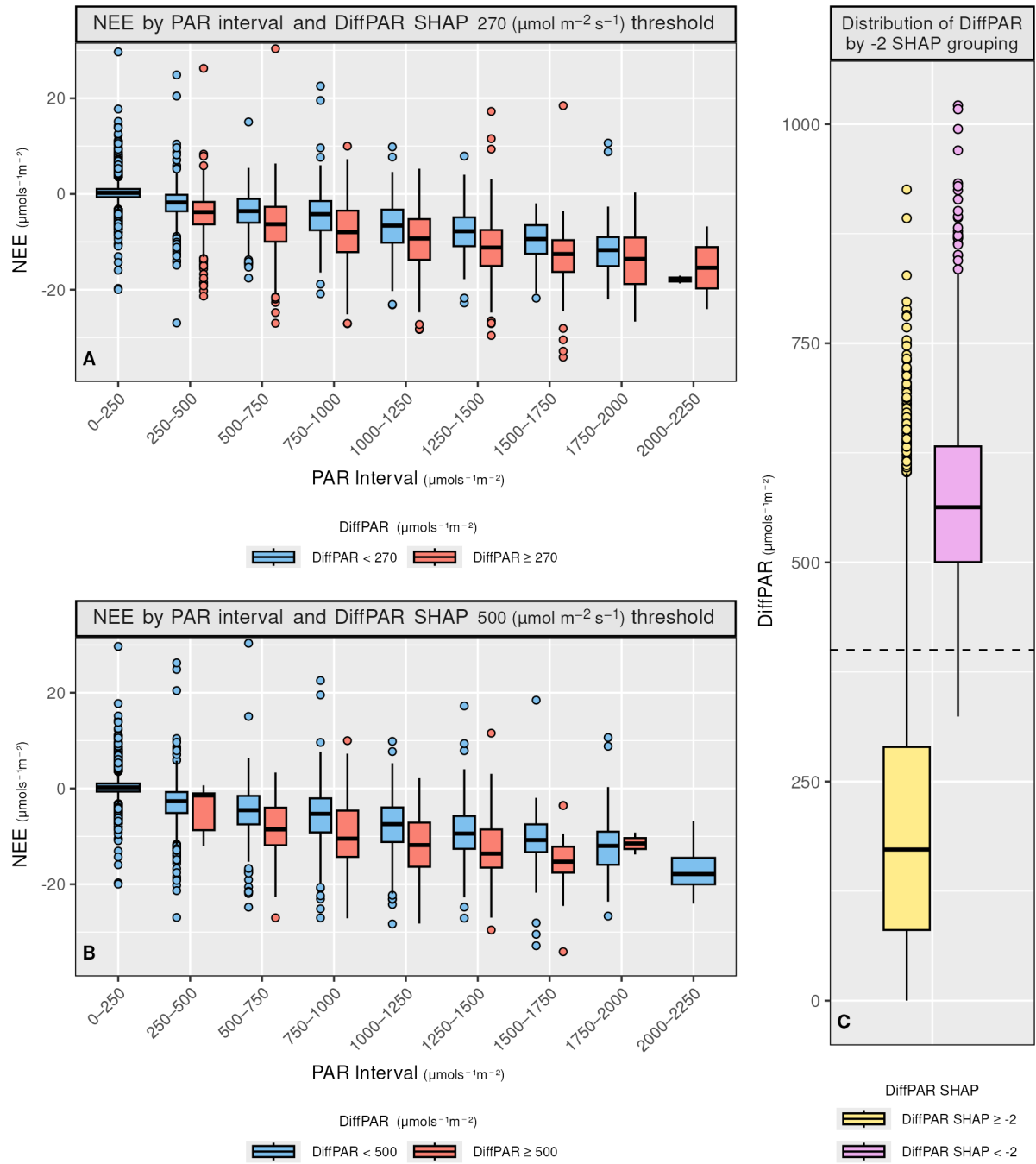
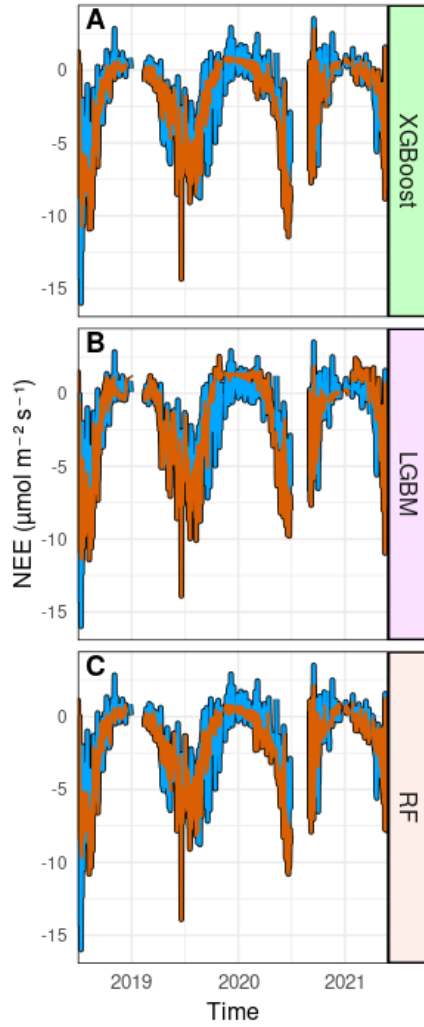


Figure A4: NEE stratified by PAR intervals using raw DiffPAR thresholds: A, 270 $\mu\text{mol m}^{-2} \text{s}^{-1}$; B, 500 $\mu\text{mol m}^{-2} \text{s}^{-1}$. DiffPAR stratified by SHAP-based grouping is shown in C.

Observed vs predicted NEE (daily mean)



Residuals and Predicted NEE, color: density

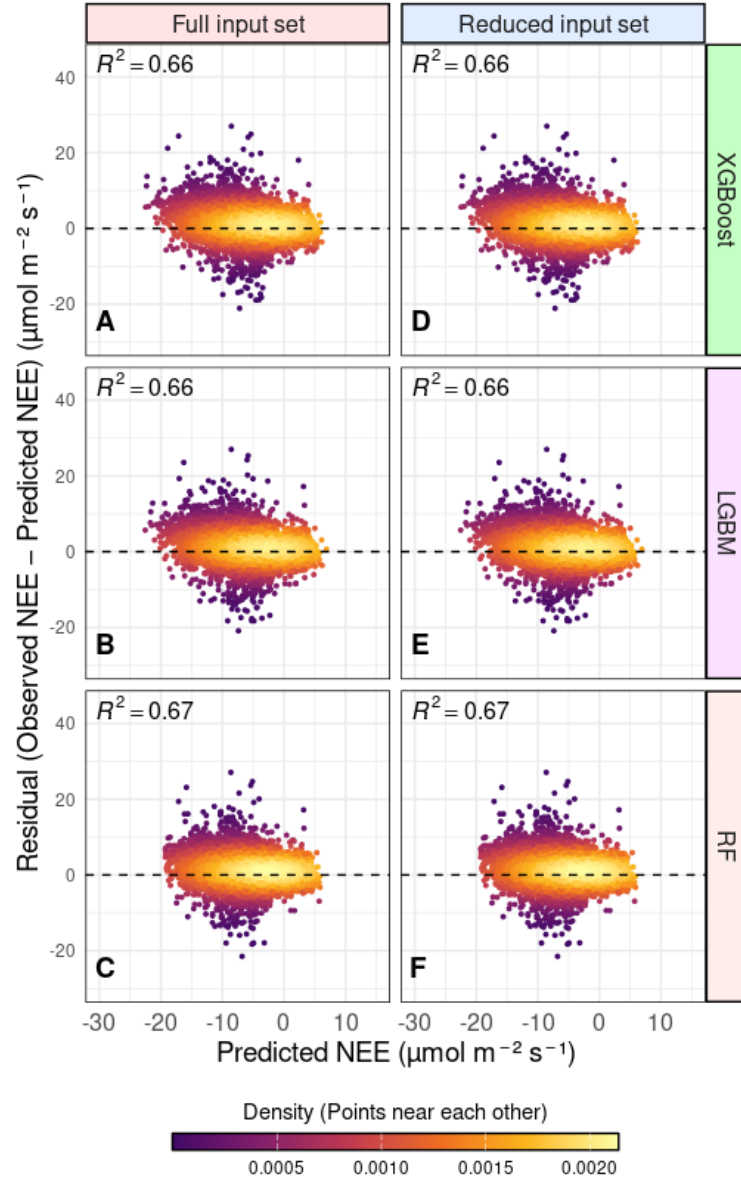


Figure A5: Observed versus predicted NEE, daily means, left, and residuals against predicted NEE, right, for the time-blocked holdout, where the earliest 75% of observations were used for training and the latest 25% for testing. Performance is lower than under the random split, but the main temporal structure is still captured.