Probabilistic Solar Proxy Forecasting with Neural Network Ensembles

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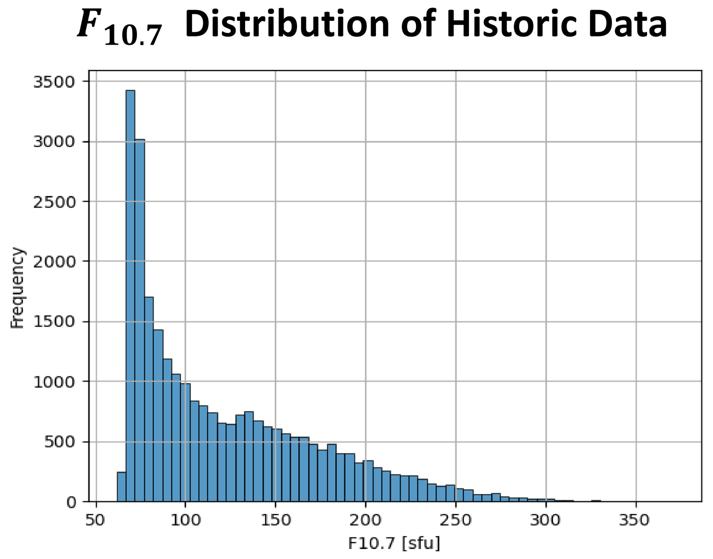
Background & Our Work

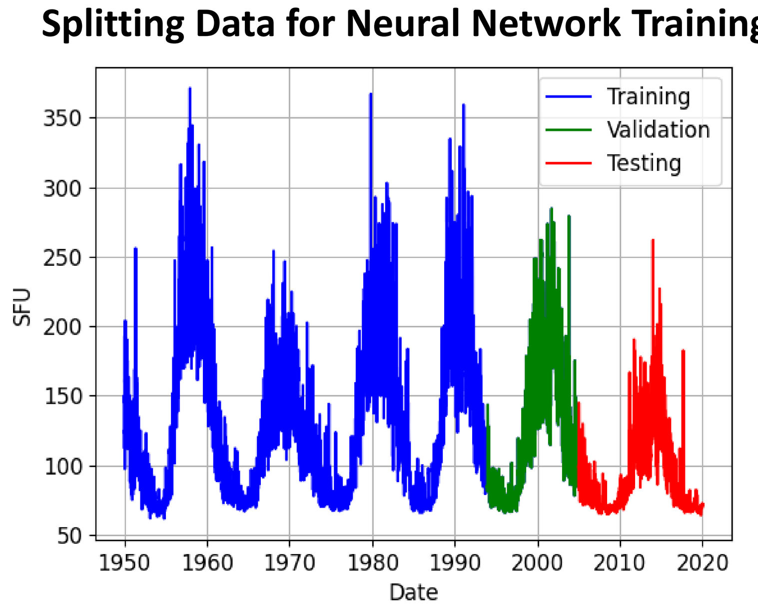
$F_{10.7\,cm}$ is an input (driver) for almost all thermosphere density models, including the operational HASDM. The thermosphere density models majorly impact satellite drag calculations. The USAF contracts a prediction of the proxy using a linear algorithm.[1] Previous non-linear *AR* methods are successful at forecasting $F_{10.7}$ but are aimed at longer term forecasting.[2] This work develops an **improved short term forecasting method of $F_{10.7}$ using neural network ensembles,** we find that the new probabilistic approach provides **significantly better relative metrics** compared against the current linear approach. Our novel work provides improvements in forecasting and includes **robust and reliable uncertainty estimation for the predicted proxy.**

Data

$F_{10.7}$ Distribution of Historic Data



Splitting Data for Neural Network Training



- †Data: (daily $F_{10.7\,cm}$ observed values) 1948-2020.
- For machine learning data splitting must be done carefully!
  - ➢ Want to maximize the size of the training set.
  - ➢ Want to include all activity levels in split sets.
- Auto-Regressive models forecast $F_{10.7}$ using only past values.

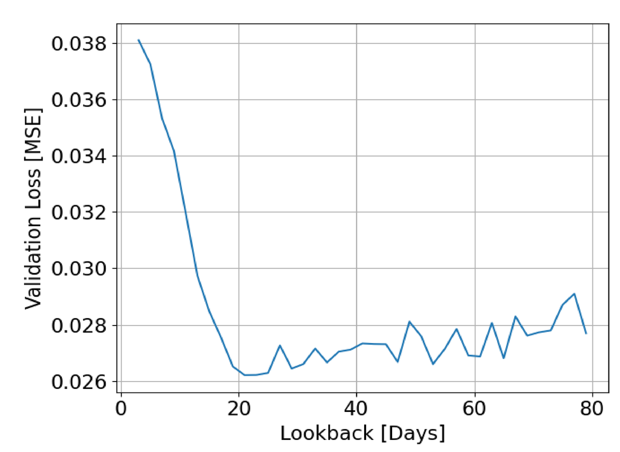
Sliding Window Approach

Forecast Epoch	Day									
Day 4	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10
Day 5	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10
Day 6	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10
Day 7	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10
Day 8	Day 1	Day 2	Day 3	Day 4	Day 5	Day 6	Day 7	Day 8	Day 9	Day 10

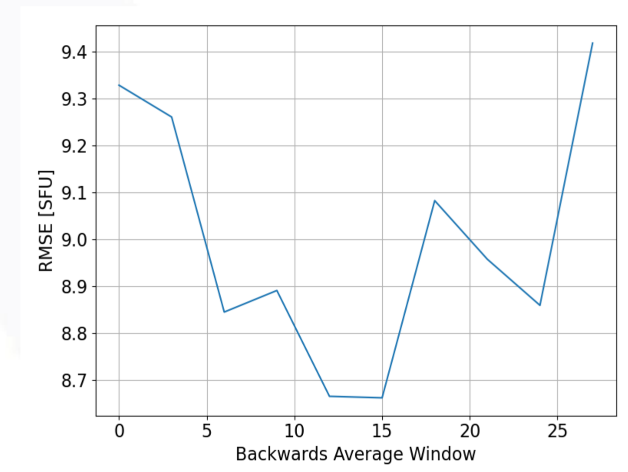
Current Day | Lookback | Horizon Values | Unused for Step

Methods: Input Investigation

Variation of Lookback



Variation of Backwards Average



- How can we extract more information, while only using historical $F_{10.7\,cm}$ data?
- *Varied Lookback*: Include variety of previous daily values as inputs to identify more trends.
- *Backwards Average*: Allows short term trend to be input to models directly.
- *AR* methods are limited by lack of varied information. We lack "the whole picture".

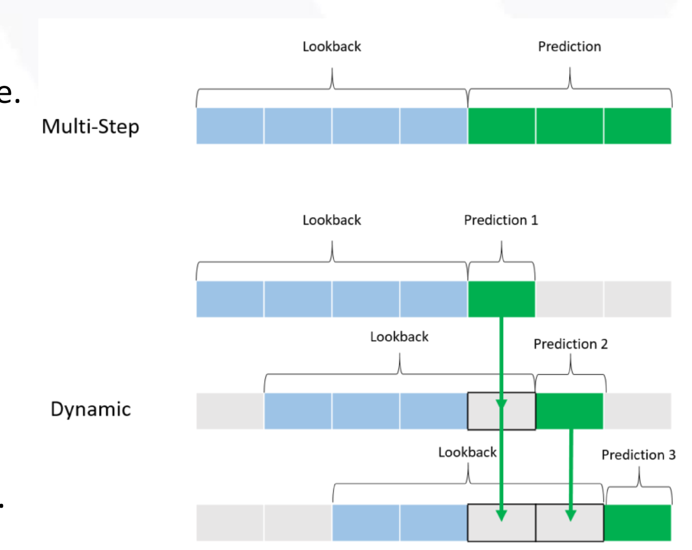
Methods: Forecasting: Multi-Step vs. Dynamic

Multi-Step

- Trained to predict multiple time steps at once.
- Prediction step occurs 1 time per day.
- Trained & limited to a fixed forecast horizon.

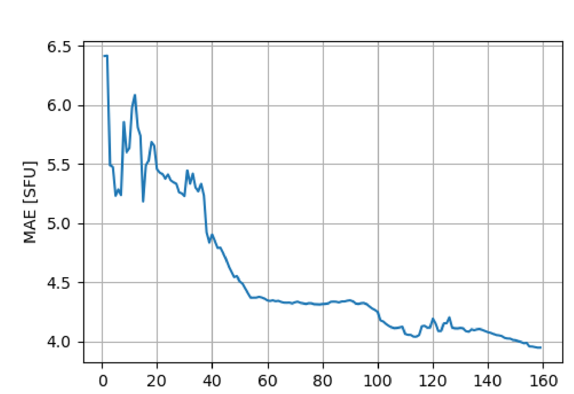
Dynamic

- Trained to predict single time step values.
- Prediction occurs recursively 6 times per day.
- Horizon can be changed during forecasting.

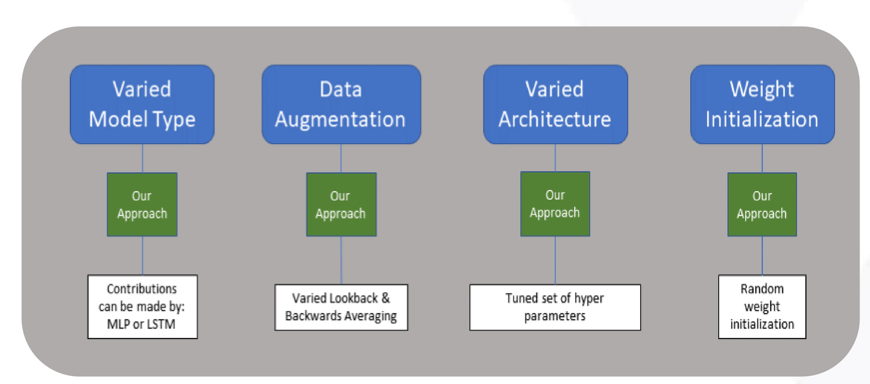


Methods: Ensembles & Diversity

Model Ensembles Decrease Error



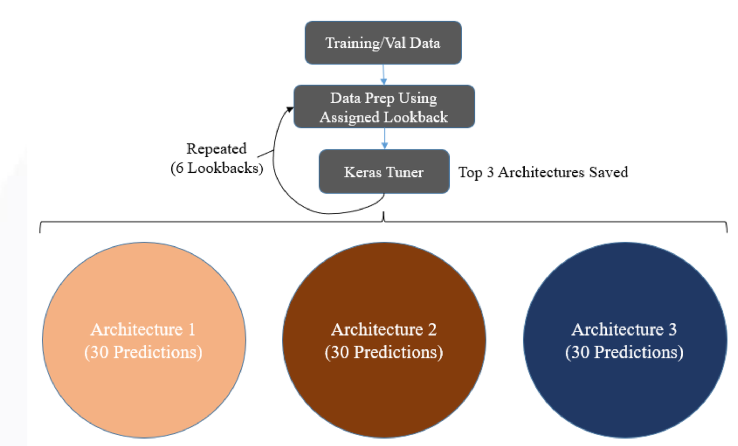
Diversity Strategies for Ensembles



- Individual model forecasts are deterministic, *model ensemble forecasts are probabilistic*.
- Ensemble members can be skilled in different areas which provides a diverse set of predictions.
- Multiple predictions are equally weighted to form an ensemble prediction, in this case 180 models.
- *A 48% decrease in MAE between 1 model and 180 models, demonstrates the skill of an ensemble.*

Methods: Neural Network Models (Ensemble Members)

Generating Ensemble Members



Tunable Hyper Parameters

MLP (Multi Layer Perceptron)

Tuner Option	Choice	Parameter	Value/Range
Scheme	Bayesian Optimization	Number of Dense Layers	[1-8]
Total Trials	100	Dense Neurons	[4-256]
Initial Points	5	Activation	[relu,tanh,sigmoid]
Repeats per Trial	3	Optimizer	[adam, SGD]
Minimization Parameter	MSE	Learning Rate	[.01, .001, .0001]
Epochs	100	Early Stopping Criteria	validation loss (MSE)
Early Stopping Patience	30		

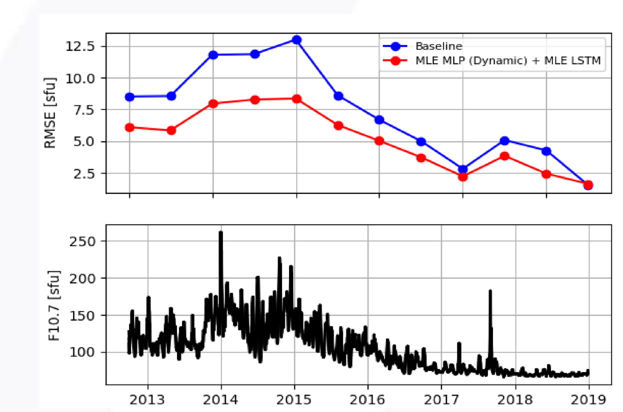
LSTM (Long-Short Term Memory)

Tuner Option	Choice	Parameter	Value/Range
Scheme	Bayesian Optimization	Number of LSTM Layers	[1-3]
Total Trials	75	LSTM Neurons	[4-128]
Initial Points	5	LSTM Activation	tanh
Repeats per Trial	3	Number of Dense Layers	[1-4]
Minimization Parameter	MSE	Dense Neurons	[4-256]
Epochs	50	Dense Activations	[relu, tanh, sigmoid]
Early Stopping Criteria	validation loss (MSE)	Learning Rate	[.01, .001, .0001]
Early Stopping Patience	10	Optimizer	[adam, SGD]

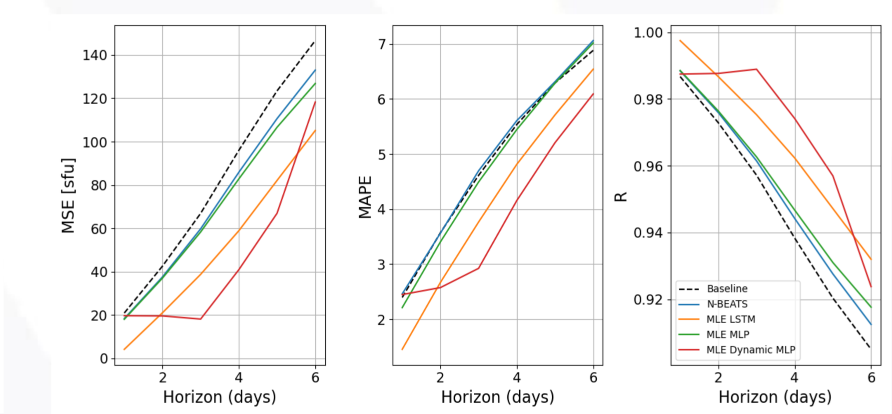
- Mean Squared Error (MSE) was used as loss function during model selection and training.
- Set of 6 lookbacks were used [7, 10, 13, 16, 19, 22 days] to promote model diversity (differing skill areas).
- The top 3 hyper parameter sets (*architectures*) are then chosen for each lookback for diversity.
  - ➢ Top 3 architecture choice made based on minimizing validation loss after hyper parameter tuning.
- 10 models of a given architecture with randomly initialized weights are trained and saved.

Results: Proxy Forecasting

Comparison of 180 Day Averaged Error



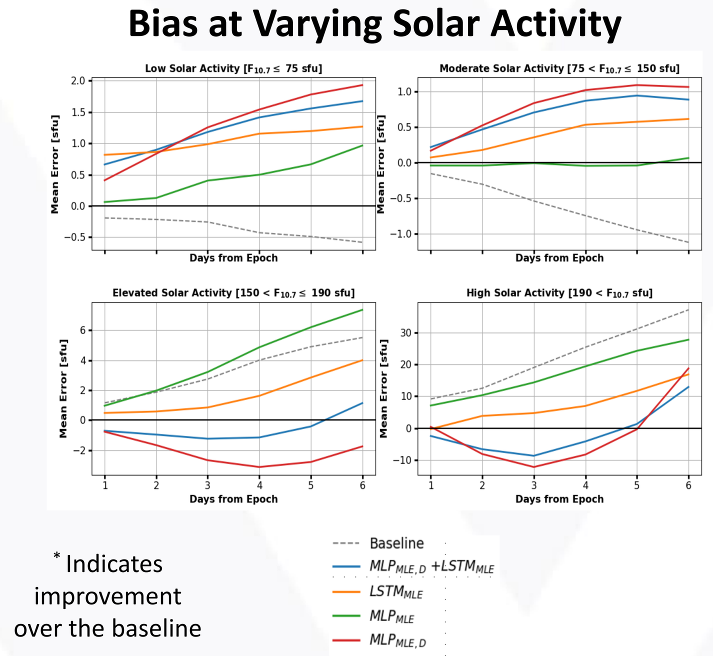
Performance Metrics Over Horizon



- Varied model types (MLP & LSTM) for predictions.
- 180 models used to form ensemble forecast.
- Ensemble methods improved performance over the baseline linear method.
- As expected, forecast error changes over time.

Model	* Relative Mean Squared Error (MSE)		
	Test (2006-2020)	*Validation (1994-2004)*	*Training Sample (1964-1974)*
$MLP_{MLE\ D} + LSTM_{MLE}$	44.2%	46.2%	55.5%

Bias at Varying Solar Activity



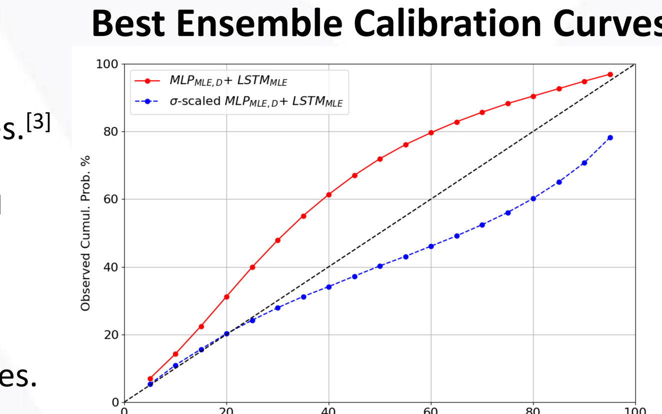
* Indicates improvement over the baseline

Results: Robustness and Reliability of Uncertainty Estimates

- Mean error (bias) indicates temporal uncertainty.
- CES quantifies uncertainty estimates made by ensembles.[3]
- σ scaling applies correction factor using validation set.[4]
- Uncertainty estimates are robust and reliable.
  - ➢ Slight under prediction seen at higher percentages.

Calibration Error Score (CES)			
Model	*Test (2006-2020)*	*Validation (1994-2004)*	*Training Sample (1964-1974)*
$MLP_{MLE\ D} + LSTM_{MLE}$	13.4%	14.34%	18.20%
$MLP_{MLE\ D} + LSTM_{MLE}$ (σ scaling)	9.8 %	5.22 %	14.51%

Best Ensemble Calibration Curves



$$\sigma_S = \sqrt{S} * \sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N} \sigma_i^{-2} * (y - \hat{y})^2} * \sigma$$

$$CES = \frac{100\%}{m}\sum_{i=1}^{m}\left|p(\alpha_j) - p(\hat{\alpha}_j)\right|$$

Conclusions

- AR data can be manipulated to improve performance.
- Mean Error (bias) is decreased at higher solar activity levels.
- NN ensemble techniques allow for probabilistic forecasting.
- Uncertainty estimates from probabilistic forecasts can be evaluated; both quantitatively and qualitatively.
- *The best NN ensemble method provided more than a 50% improvement over SET's linear forecasting method.*

Future Work

- Investigate advanced ensemble combination techniques.
  - ➢ Temporal debiasing
  - ➢ Performance based weighting
- Apply ensemble techniques to other space weather indices and/or proxies.
  - ➢ Simultaneous multivariate forecasting
- Investigate te coupling of different sources of uncertainties.
  - ➢ Model uncertainty & Driver uncertainty

References

[1] Licata, R. J., Tobiska, W. K., & Mehta, P. M. (2020). "Benchmarking forecasting models for space weather drivers." (2020).

[2] Stevenson, Emma et al. "A deep learning approach to solar radio flux forecasting." (2022).

[3] Licata, R. J., et al. "Machine-learned HASDM thermospheric mass density model with uncertainty quantification." (2022).

[4] Laves, Max-Heinrich, et al. "Recalibration of Aleatoric and Epistemic Regression Uncertainty in Medical Imaging." (2021).

Acknowledgements

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