Uncertainty Quantification for Ionosphere Forecasting with Machine Learning

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IWGI2022 - Observations, Modelling and Applications

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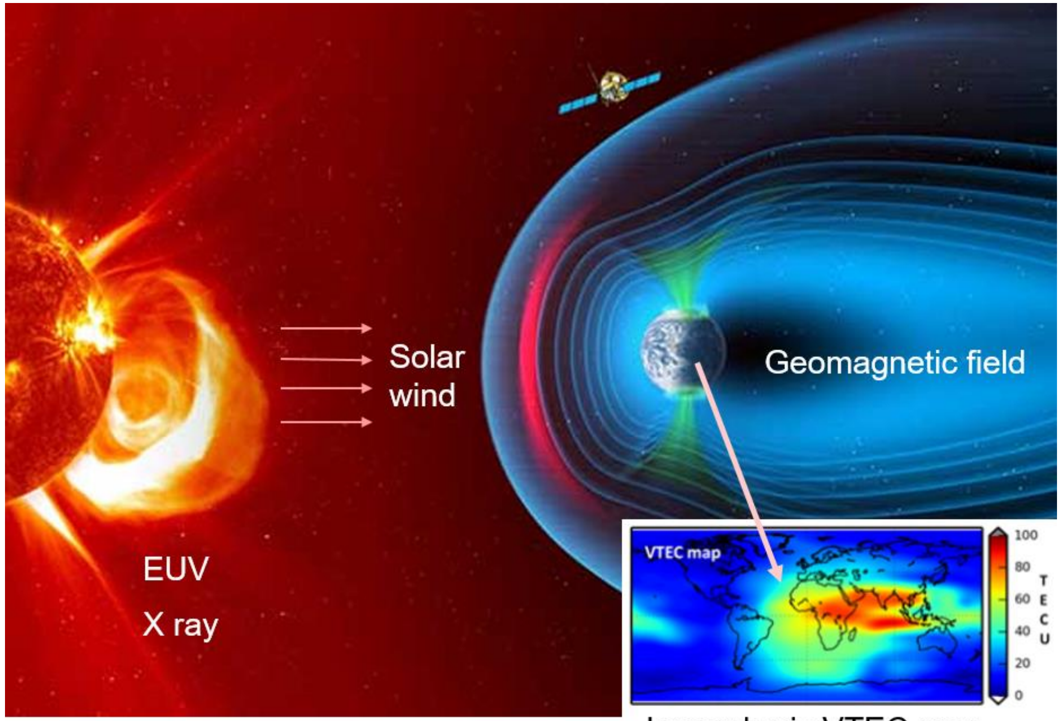
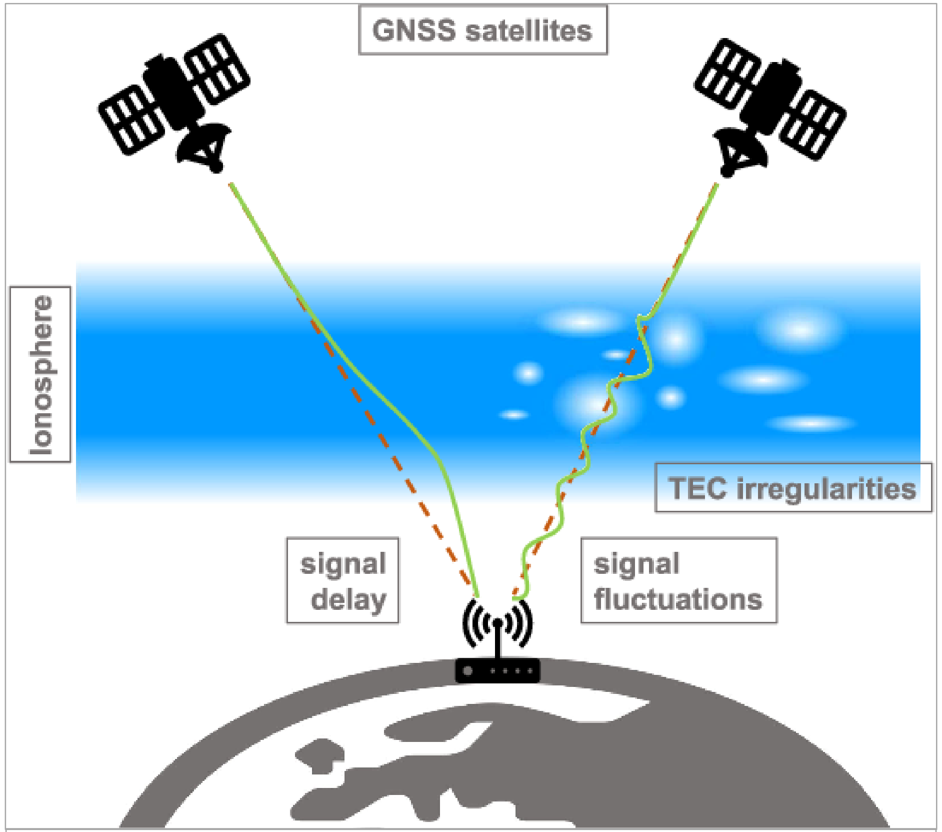
Research problem

- ➢ Ionospheric refraction of GNSS signals
- ➢ Dual-frequency observations → integrated electron density (STEC)
- ➢ Vertical Total Electron Content (VTEC)



Ionospheric VTEC map

Image source: ESA (background), DGFI-TUM (VTEC map).

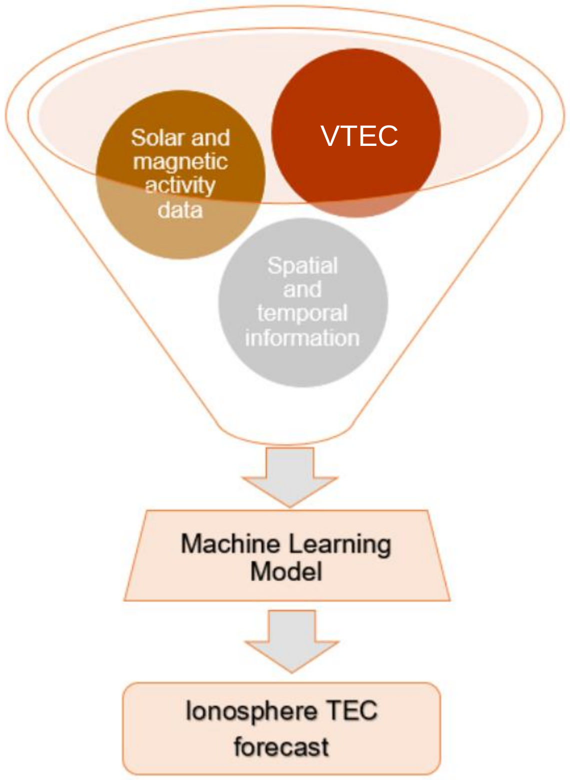


Source: https://www.semanticscholar.org/paper/Detection-of-GNSS-Ionospheric-Scintillations-Based-Linty-Farasin/3bc53da7342d4cdcd1a8bacfdc92651aeb62d5dc

Research problem

Objectives:

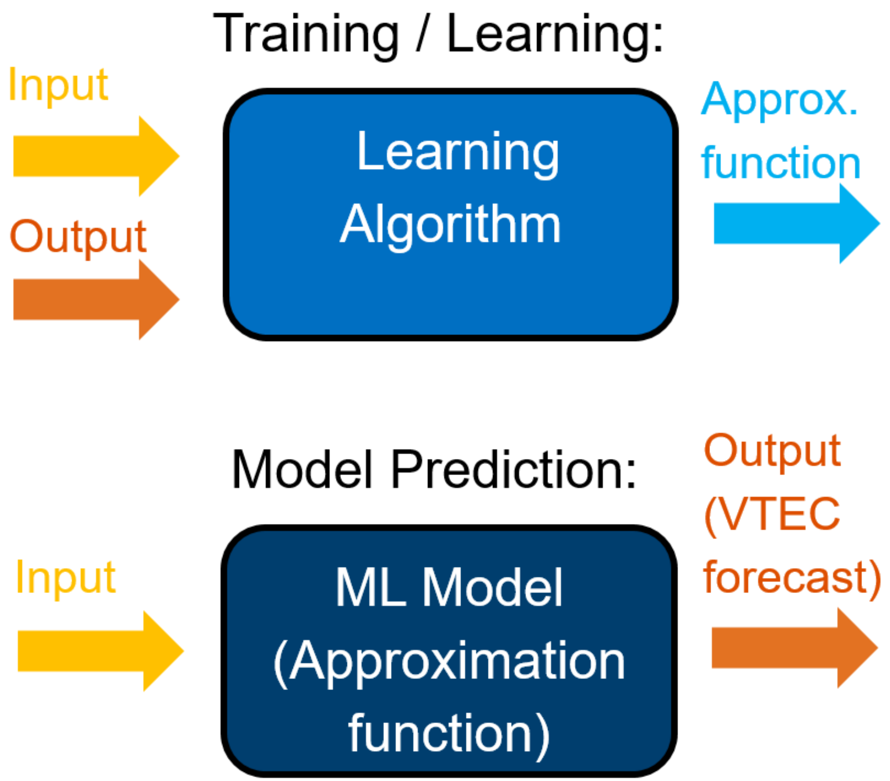
- ➢ Model / forecast VTEC accurately and precisely
  - ➢ Including solar-terrestrial processes (space weather)
  - ➢ How certain and reliable are the predictions



Machine learning (ML):

- ➢ “Learning” from the data
- ➢ Approximating nonlinearity

Supervised learning



Natras and Schmidt (2021), *CEUR Workshop Proceedings*
http://ceur-ws.org/Vol-3052/short10.pdf

Uncertainty quantification (UQ)

- ✓ How confident and accurate are decisions from an AI-based system?
- ✓ ”Uncertainty-aware” predictions
- ✓ Produce the model output in a probabilistic framework
- ✓ Define the accuracy and precision of VTEC prediction
- ✓ Quantify the level of trust in VTEC prediction
- ✓ Quantify the level of reliability with confidence intervals
- ✓ Important for forecasting and decision making

1-day VTEC Forecasting, Data (time sampling 1h)

Input data:

Time: t

- Time: Hour of day and Day of year (DOY)
- Sunspot number R (daily)
- Solar radio flux F10.7 (daily)
- Solar wind plasma speed (hourly)
- Bz index (hourly)
- AE index (hourly)
- Dst index (hourly)
- Kp index (3-hour)
- VTEC from GIM CODE (hourly)
  - 10°E 70°N, 10°E 40°N, 10°E 10°N
- Exponential moving average of VTEC over previous 4 days and 30 days
- First time derivative of VTEC
- Second time derivative of VTEC

GIM CODE VTEC as ground truth (GT) → non-error free

Output data:

- VTEC
  - 10°E 70°N,
  - 10°E 40°N,
  - 10°E 10°N

Time: t+24h

Data split:

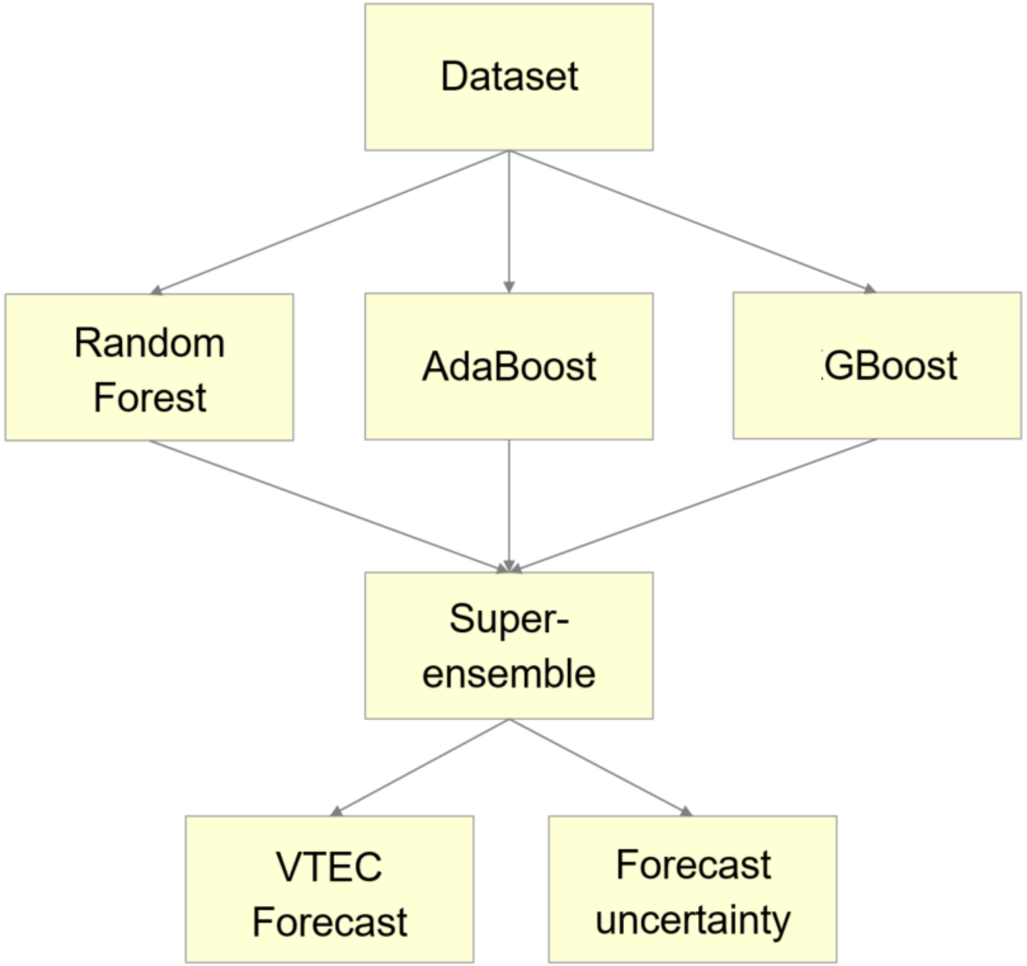
- Training & Cross-validation: 2015 - 2016
  - Cross-validation on a rolling basis
- Test: 2017

Natras et al. (2022), *Remote Sensing*
https://doi.org/10.3390/rs14153547

Uncertainty quantification (UQ)

I. Multi-model and multi-data ensemble

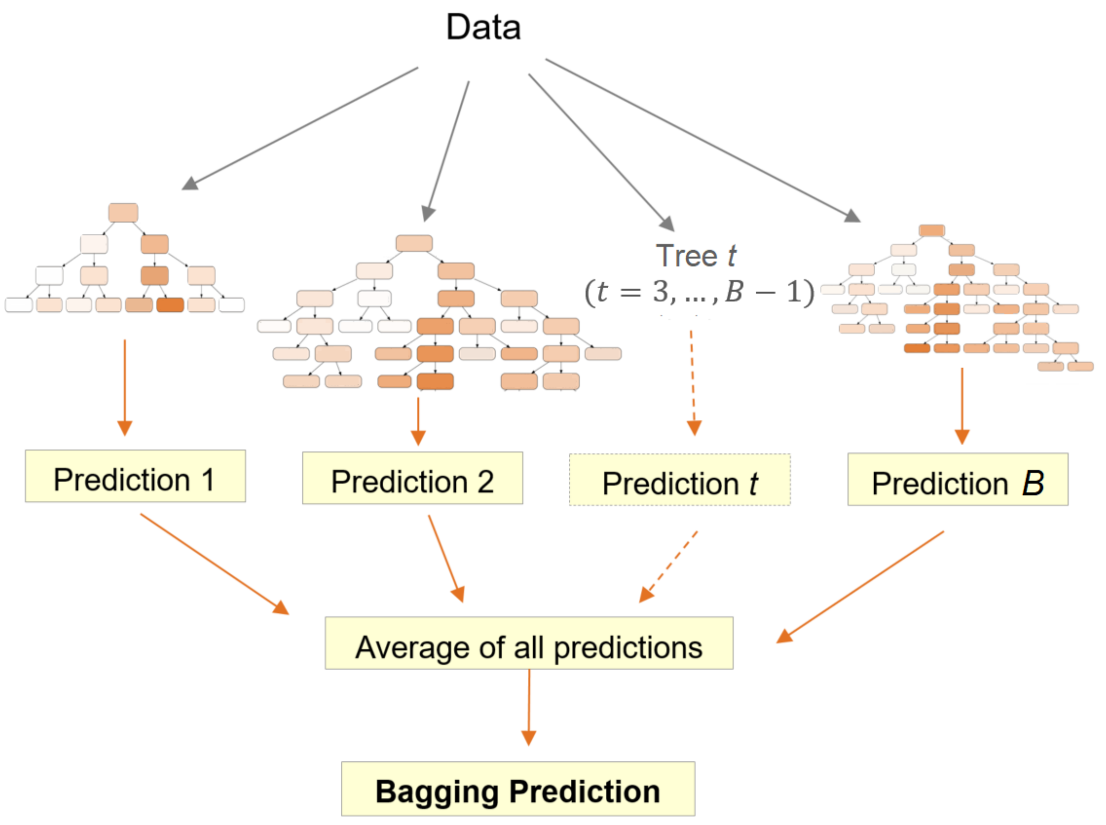
- Super ensemble (**SE**)
- VTEC forecast → ensemble mean
- Forecast uncertainty → ensemble spread (2σ)
- 3 datasets*:
  1. d1: original data in input and output
  2. d2: daily differences in input and output
  3. d3: Input: d1 + d2, output: d2



*Observations were preprocessed / cleaned before training.

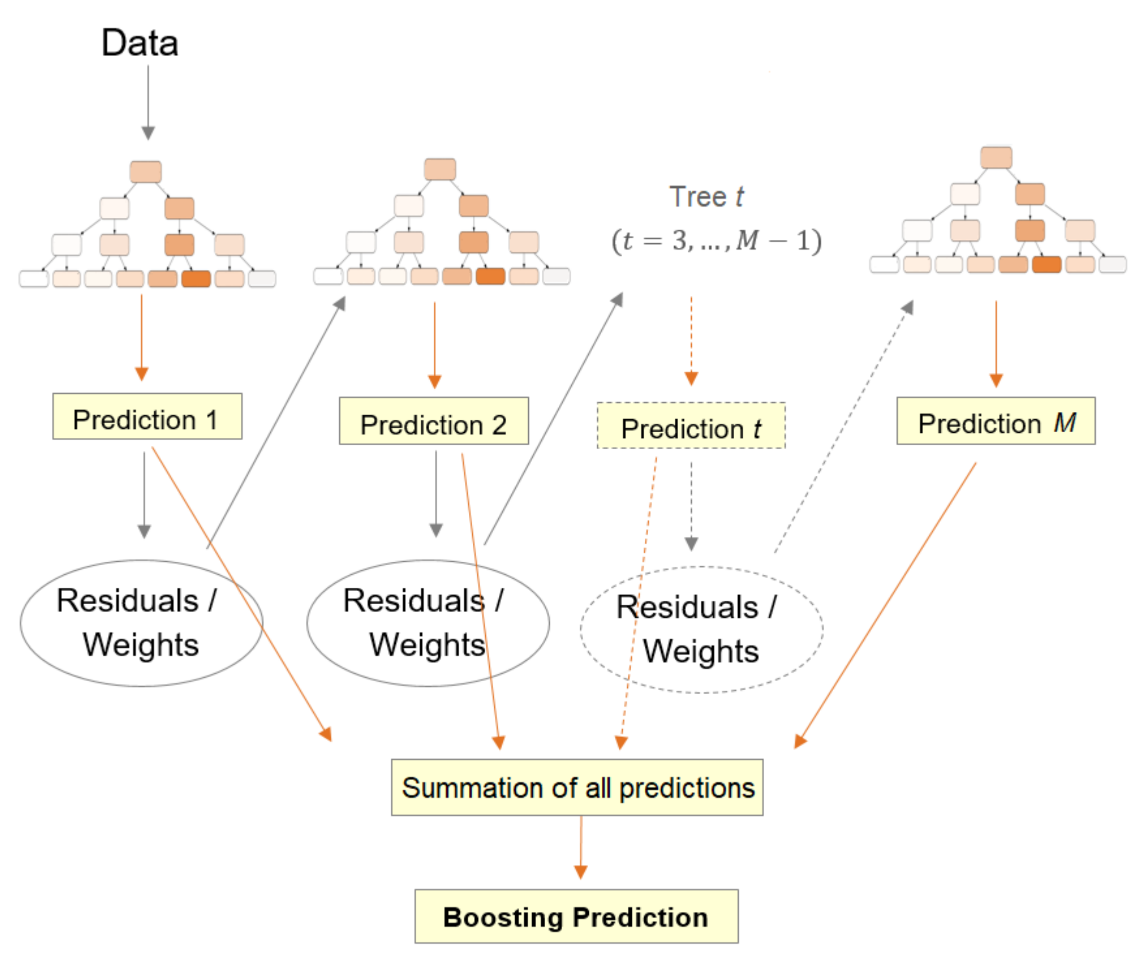
Natras et al. (2022), *3rd URSI AT-AP-RASC*
[10.23919/AT-AP-RASC54737.2022.9814334](https://doi.org/10.23919/AT-AP-RASC54737.2022.9814334)

Tree-based learning



- **Bagging** (Parallel learning):
  - Random Forest (multiple randomized trees)

- **Boosting** (Sequential learning)**:**
  - Adaptive Boosting AdaBoost (training with weighted obs.)
  - Gradient Boosting GBoost (training with residuals)



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Uncertainty quantification (UQ)

II. Quantile confidence interval

- Quantile objective loss function
- Applied for GBoost and dataset d1 → Quantile Gboost (**QGB**)

$$\mathcal{L}(e_i|\beta) = \begin{cases} \beta e_i & \text{if} \quad e_i \geq 0, \\ (\beta - 1)e_i & \text{if} \quad e_i < 0 \end{cases} \qquad e_i = y_i - \widehat{y_i}$$

$$\mathcal{L}(\mathbf{e}|\beta) = \frac{1}{N}\sum_{i=1}^{N} \mathcal{L}(e_i|\beta)$$

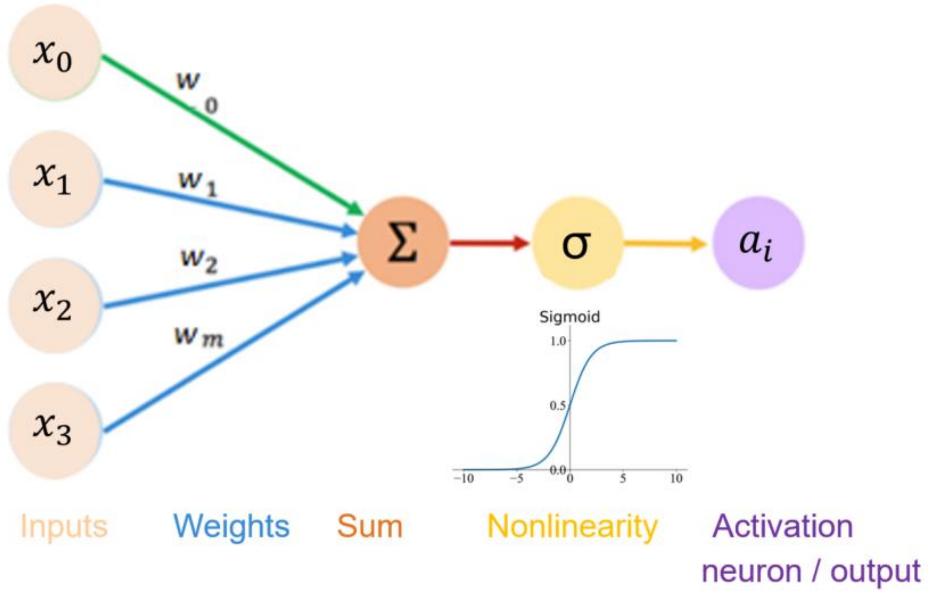
- β value of a quantile
- Quantiles: upper bound $\beta = 0.95$, lower bound $\beta = 0.05$
- 90% predicted confidence interval

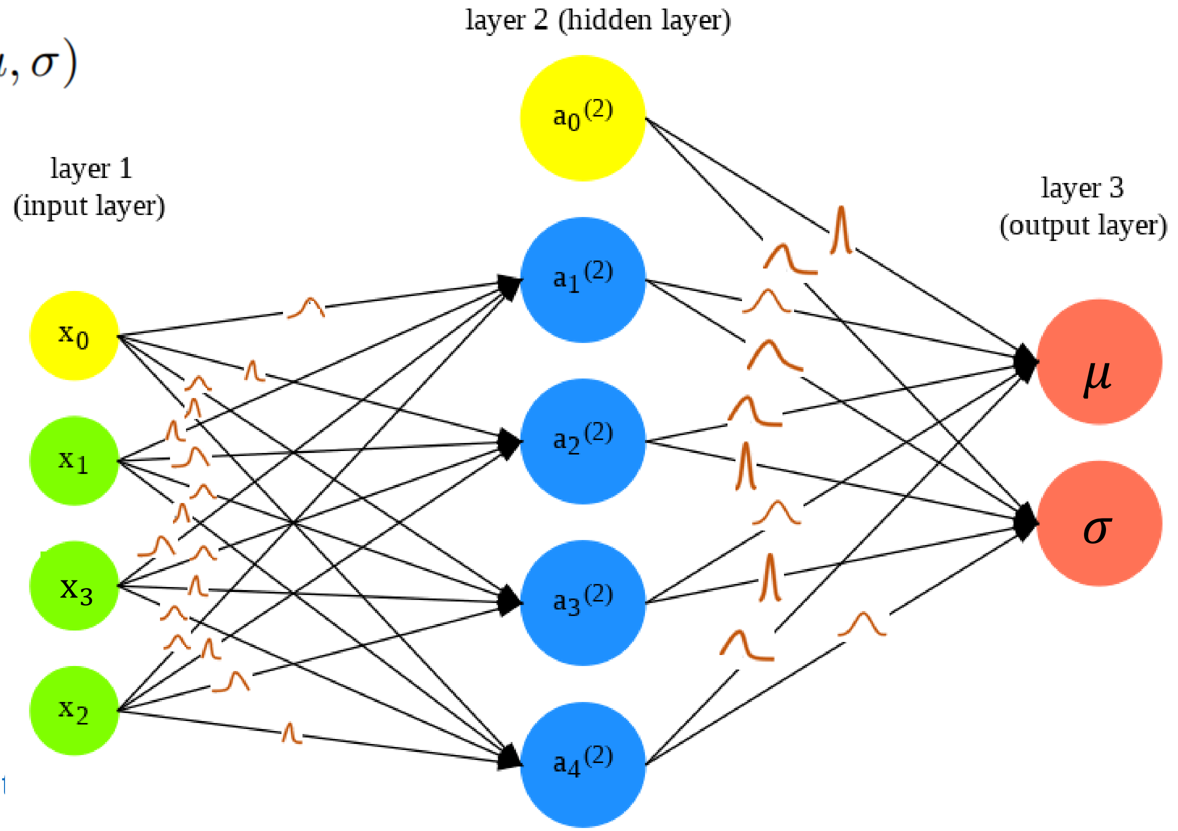
Uncertainty quantification (UQ)

III. Bayesian neural network (BNN)

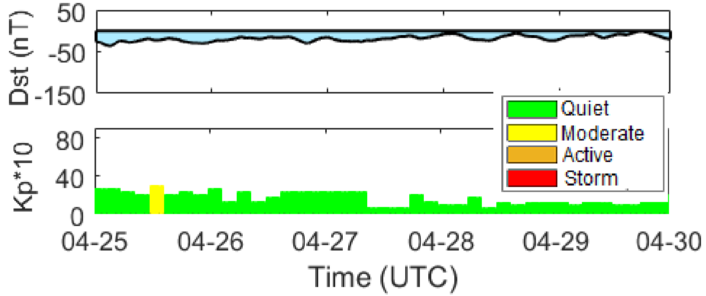
- Learning probability distributions over weights via variational Bayesian inference
- Probabilistic BNN → Negative log likelihood (NLL) loss
- Dataset d1

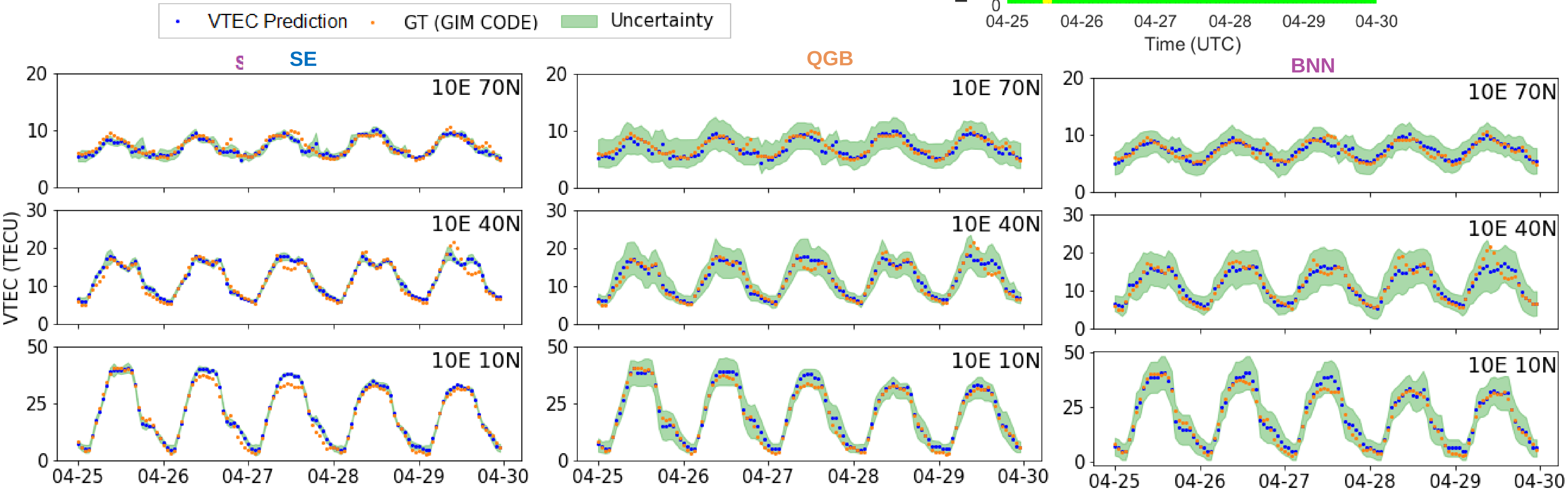
$$\mathcal{L} = -\frac{1}{N}\sum_{i=1}^{N} \log l\left(y_i|\mu,\sigma\right)$$

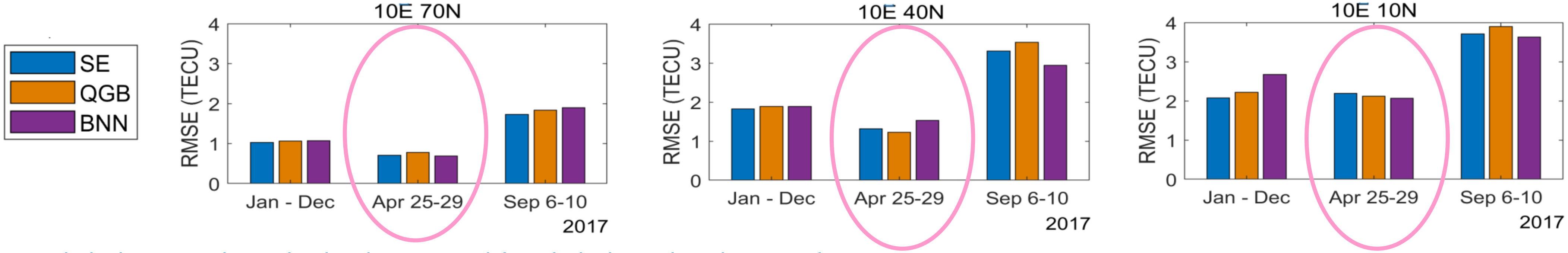




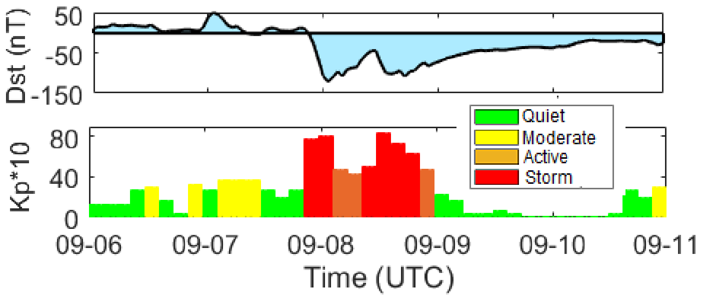
Results: Apr 25-29, 2017 (quiet)

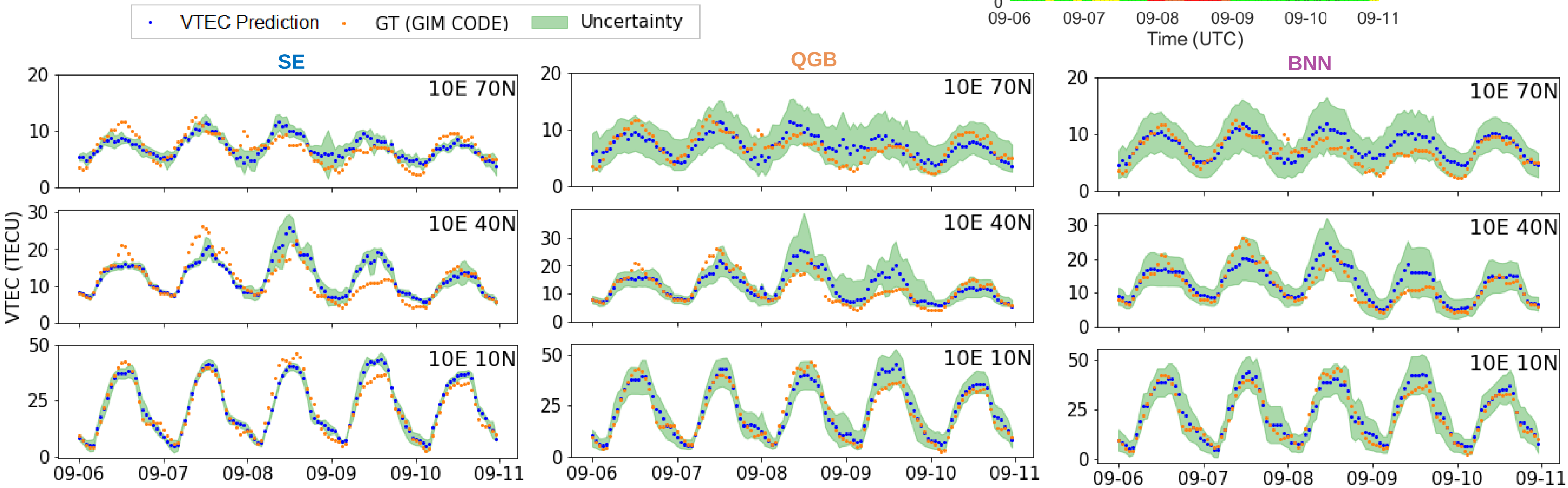


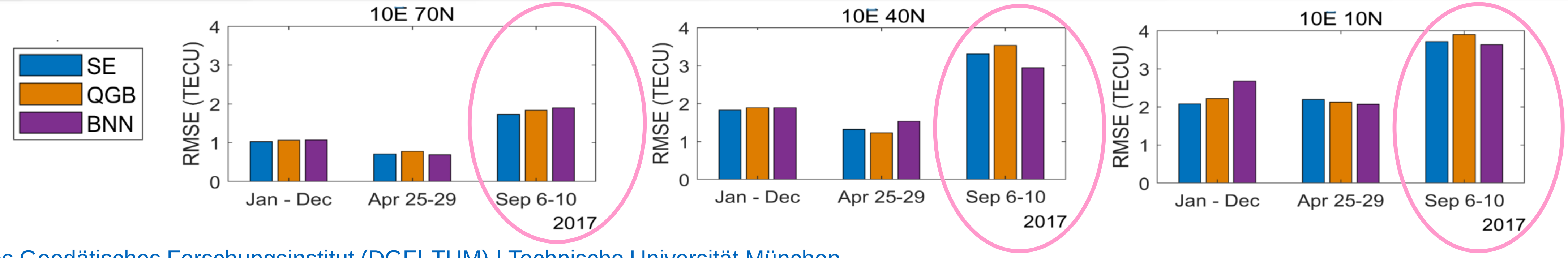




Results: Sep 6-10, 2017 (storm)







- The uncertainty information defines the reliability and precision of VTEC predictions
- UQ allows to assess the trustworthiness of predictions
- Ground-truth VTEC mostly within predicted confidence intervals of QGB and BNN
- SE: small ensemble spread → higher confidence in the forecast
- QGB and BNN: wider confidence intervals → more realistic and reliable

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(1) Natras, R.; Soja, B.; Schmidt, M. Ensemble Machine Learning of Random Forest, AdaBoost and XGBoost for Vertical Total Electron Content Forecasting. Remote Sens. **2022**, 14, 3547, https://doi.org/10.3390/rs14153547

(2) Natras, R., Soja B., Schmidt, M. "Machine Learning Ensemble Approach for Ionosphere and Space Weather Forecasting with Uncertainty Quantification", *3rd URSI AT-AP-RASC*, **2022**,1-4, 10.23919/AT-AP-RASC54737.2022.9814334

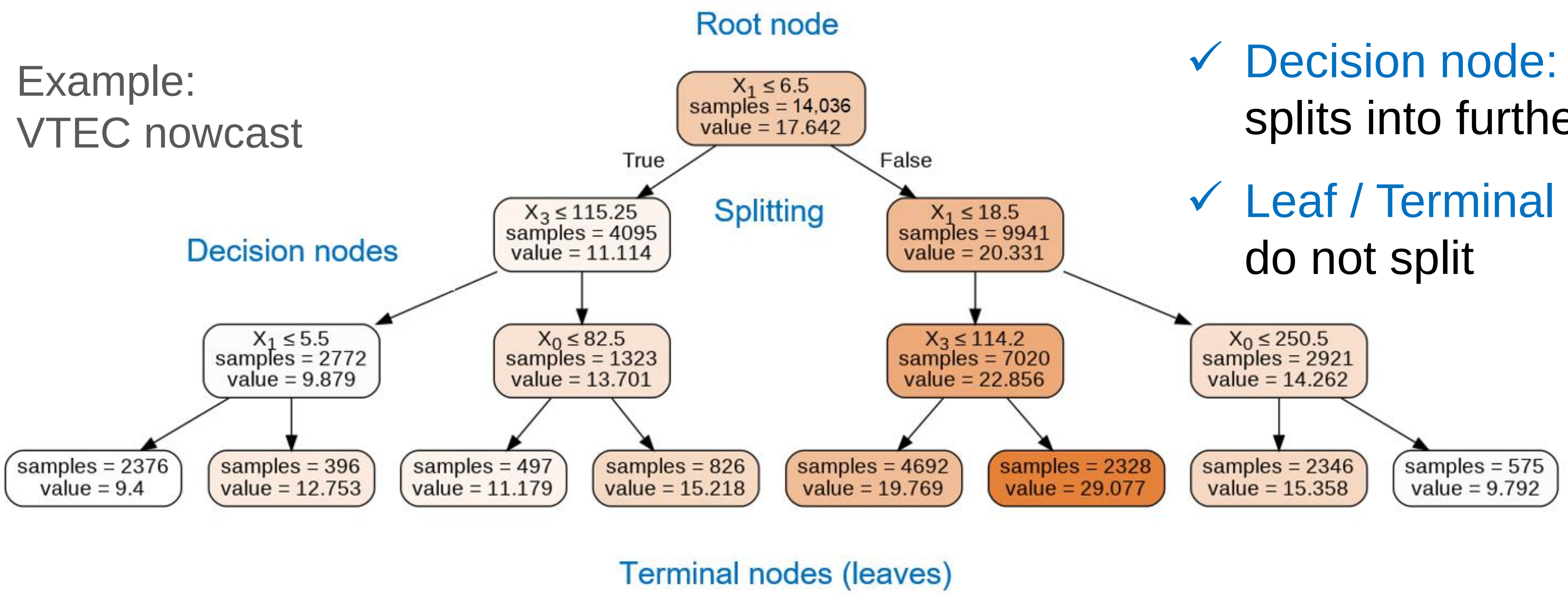
(3) Natras, R., Schmidt, M. "Machine Learning Model Development for Space Weather Forecasting in the Ionosphere", CEUR Workshop Proceedings, 3052, **2021,** http://ceur-ws.org/Vol-3052/short10.pdf

Back-up slides

Decision tree learning

Natras et al. (2022), *Remote Sensing*
https://doi.org/10.3390/rs14153547

Example:
VTEC nowcast

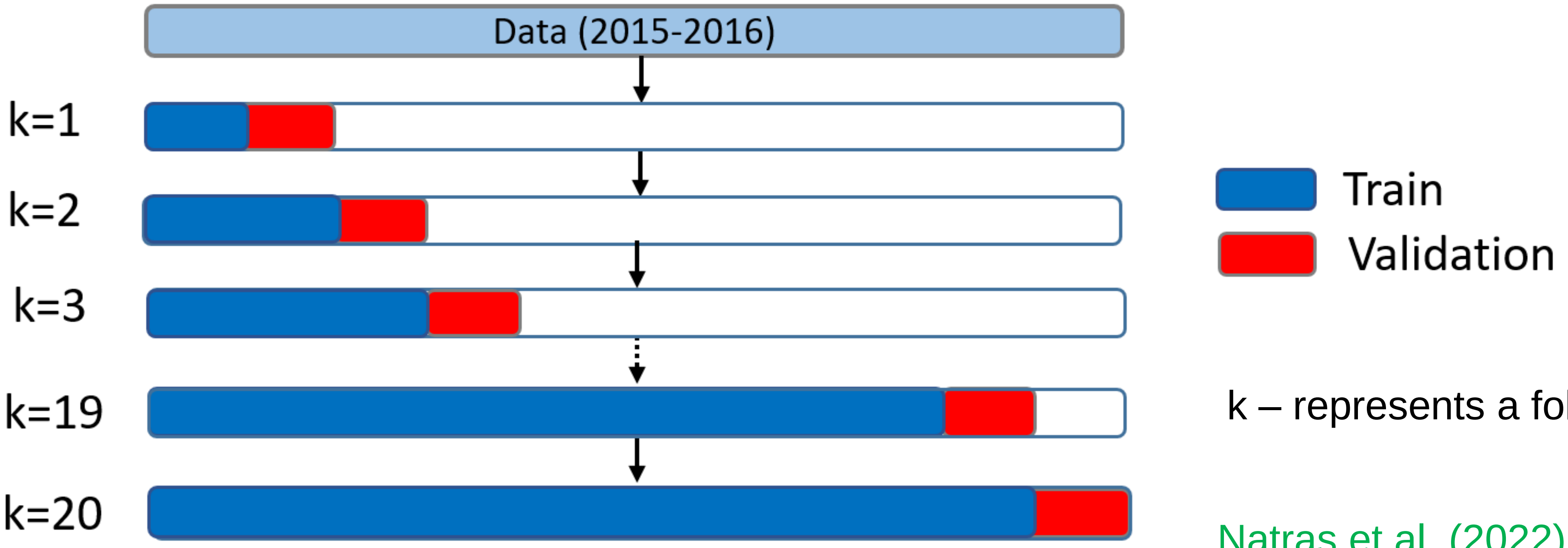


Final outcome: average VTEC in the particular leaf node.

- ✓ Root node: entire dataset; further divided into 2 subnodes
- ✓ Decision node: a subnode that splits into further subnodes
- ✓ Leaf / Terminal node: nodes that do not split
- ✓ Splitting: dividing a node into 2 subnodes by calculating reduction in variance

Model training and evaluation

- Temporal structure of time series -> cross-validation on a rolling basis
- Evaluate model performance in a robust way
- **Final metrics:** average of RMS from every cross-validation iteration (k-fold).



k – represents a fold

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Results ensemble members:

September 2017 space weather events