

THEORETICALLY INFORMED MACHINE LEARNING (ML) MODELS FOR PREDICTING PESTICIDE LEACHING IN NEW YORK (August 2025, NABEC)

Isaiah Guenther, Tammo S. Steenhuis, and others of Soil & Water Lab,
Biological and Environmental Engineering Dept. - Cornell University
With and for New York State Department of Environmental Conservation (NYSDEC), Bureau of Pesticide Management



BACKGROUND

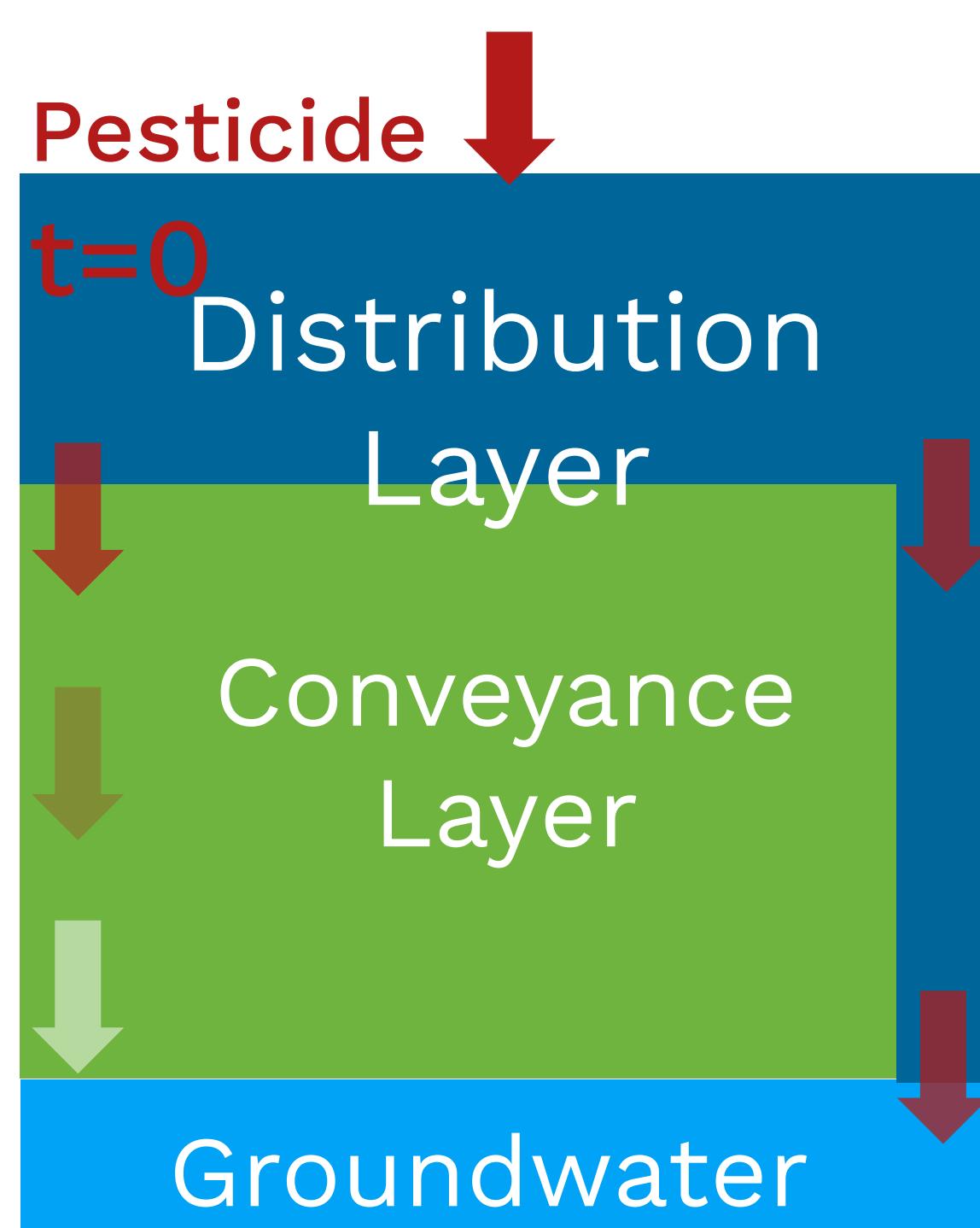
- Eastern Long Island 1970s insecticides in groundwater.
- Upstate diversely different from Long Island.
- Many eclectic pesticides and uses. Complex to forecast groundwater occurrence.
- Many non-detect results in monitoring.

Objectives

- Develop ML model that predicts leaching.
- Compare ML to theoretical model, same inputs.

MODELS AND DATA

Theoretical Groundwater Ubiquity Score (TGUS) [1]



$$t_{LRP} = \frac{t_1}{\frac{2}{\lambda}} \ln \left(\frac{\lambda \Phi}{K_{oc} f_{oc} \rho} \right)$$

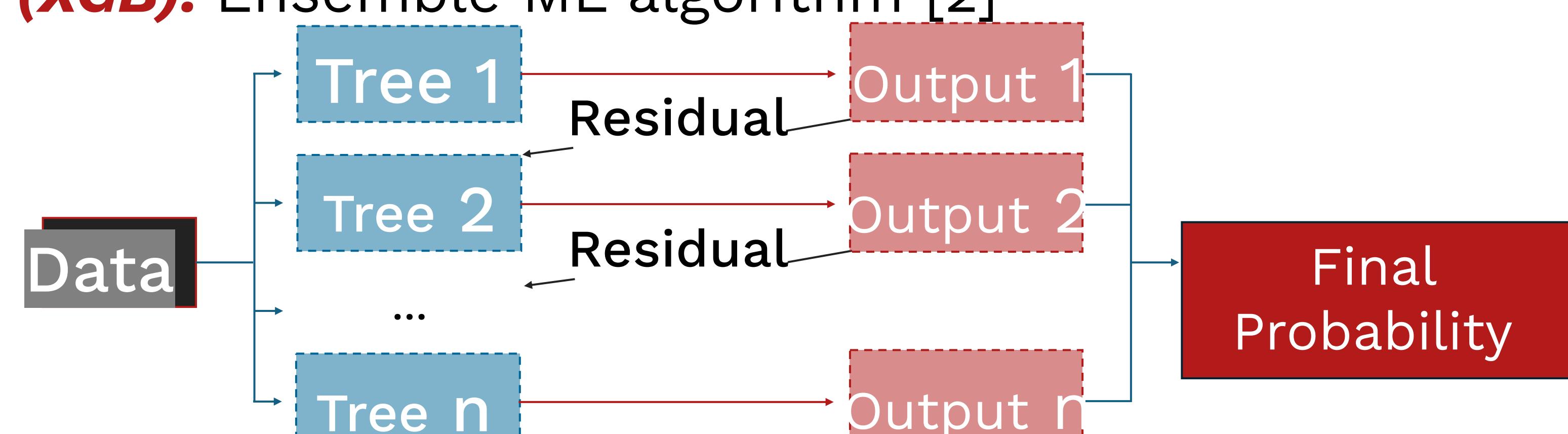
$t_1 = \text{soil halflife}[days]$,
 $\lambda = \text{preferential flow fraction}$

$\Phi = \frac{\text{application rate}}{\text{detection limit} * \text{distribution layer thickness}}$

K_{oc} = organic carbon sorption partition coeff. $\left[\frac{ml}{g} \right]$,
 f_{oc} = soil organic carbon fraction,
 ρ = soil bulk density $\left[\frac{Mg}{m^3} \right]$

Machine Learning – Extreme Gradient Boosting (XGB)

Ensemble ML algorithm [2]



XGB classification flowchart. Final class probability is the sigmoid function applied to the sum of N log-odds outputs from each tree.

Data sources and selection

- Long Island groundwater analytical data (USGS [3]), 1832 cases and NYSDEC lab upstate, 761 cases.
- USDA NRCS soil surveys, NYSDEC Pesticide Sales and Use Reporting (PSUR), pesticide product labels, and pesticide properties databases and literature.
- Cases omitted for missing chem properties and Long Island analytes with pesticide use+sales <50 lb over 6 years in zip code.

REFERENCES AND CREDITS

[1] Steenhuis, T. S., et. al. 2024.. J. of Hydrology and Hydromechanics. DOI: 10.2478/johh-2024-0016

[2] Chen, T. & Guestrin, C. 2016. DOI: 10.48550/arXiv.1603.02754

[3] Fisher, I. J., et. al. 2021. DOI: 10.1016/j.scitotenv.2020.141895

Algorithm and ML coding: Isaiah Guenther, Steven Pacenka

Database: Steven Pacenka, Naaran Brindt, Xin Shen, Xingliang Cao, Xiyue Luo, Yuchen Tao

TGUS theoretical formula: Tammo Steenhuis

Principal investigators: Tammo Steenhuis, Brian Richards

Poster: Isaiah Guenther, Steven Pacenka, Yuchen Tao.

Special thanks to Scott Stein Schneider for ML advice.

Soilandwaterlab@cornell.edu

MODEL APPLICATION

TGUS	Predict leaching with t_{LRP} : $\text{pred.} = \begin{cases} \text{detect}, & t_{LRP} \geq 100 \text{ days} \\ \text{nondetect}, & t_{LRP} < 100 \text{ days} \end{cases}$		
ML: XGB	<ol style="list-style-type: none"> CV train on 80% stratified data split. tune hyperparameters/threshold. Select “fold” with max F1. Test prediction performance on 20% held-out data set. Repeat 50 iterations steps 2-3, record all predictions and metrics 		

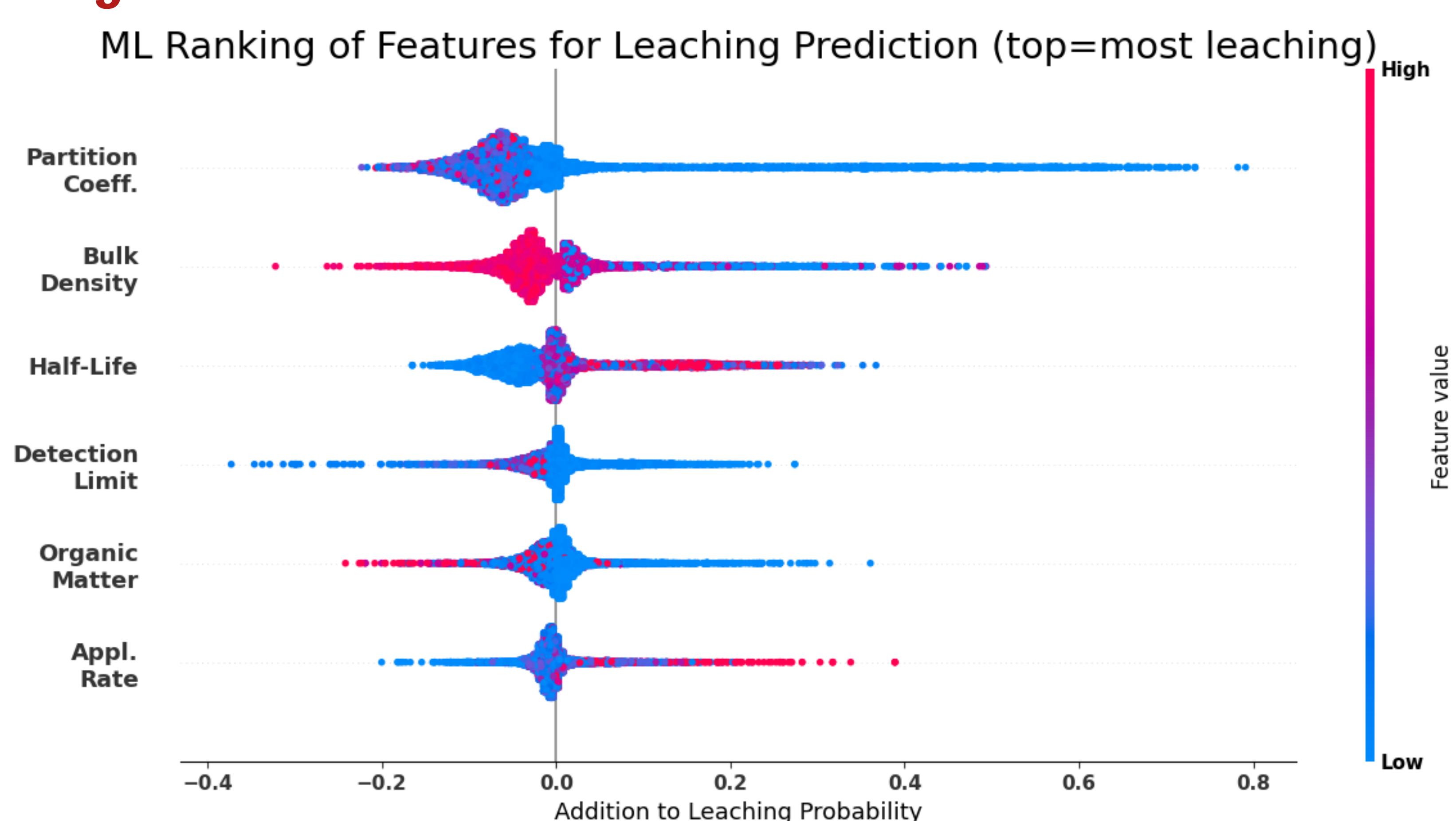
RESULTS

Model	Performance Metrics (train/test)		
	Precision [%]	Recall [%]	F_β [%]
TGUS Upstate (untrained)	-/20	-/99	-/56
XGB, upstate 6 vars	77/83	80/95	79/92
TGUS Long Isl. (untrained)	-/21	-/74	-/49
XGB, Long Island 6 vars	52/58	79/89	71/80

$$\text{Precision} = \frac{TP}{TP + FP} \quad \text{Recall} = \frac{TP}{TP + FN} \quad F_\beta = (1 + \beta^2) * \frac{\text{Precision} * \text{Recall}}{(\beta^2 * \text{Precision}) + \text{Recall}} \quad \beta = 2$$

Performance metrics from model outcomes: true positive (TP), false positive (FP), true negative (TN), false negative (FN).

Shapley beeswarm plot, six variable XGB model, upstate 20% testing dataset



left=lower effect, right=higher, blue=low variable, red=high variable

Conclusions

- XGB outperformed TGUS in most metrics, both locales.
- XGB learned patterns consistently with TGUS theory. This may corroborate TGUS method.

Considerations

- Limited datasets and empirical scope of ML tools.
- No analysis of feature interactions (yet).
- Two of eight TGUS params not readily available.