Interpretable and Uncertainty-aware Neural Networks

Prasad Deshpande and Sourajit Dey
Digital Agronomy Research Team
deshpande@ksu.edu and sdey@ksu.edu

KANSAS STATE UNIVERSITY

Pre-workshop assessment

https://tinyurl.com/mlunicamp25post

DART
DIGITAL AGRONOMY RESEARCH TEAM

Machine Learning: Introduction

Machine Learning (ML):
Training computers to **learn patterns** from data to make predictions.

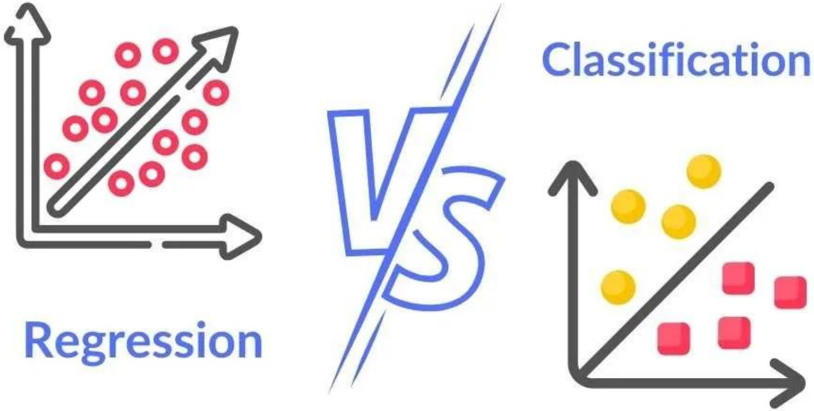
Analogy:

- Traditional Programming:
  - Data + Rules → Output
  - If rainfall < 50 mm and NDVI < 0.3, then predict "Low yield"
- Machine Learning:
  - Data + Output → Learn Rules → Predict on New Data
  - We don't write the rules – the algorithm learns them from examples

Machine Learning: Introduction

Types relevant to agriculture:

- Regression:
  - Numerical output
  - Example: yield prediction
- Classification:
  - Categorical output
  - Example: classify crop type from images



DART
DIGITAL AGRONOMY RESEARCH TEAM

Machine Learning: Supervised learning

The model learns from **labeled data** (correct answer is known), i.e., targets

Data contains:

- **Features (inputs)**: Variables used to make predictions
- **Target (output)**: What we want to predict

Example: **Yield Prediction**

- **Features**: NDVI, rainfall, temperature, soil type
- **Target**: crop yield (kg/ha)

Machine Learning: Unsupervised learning

- The model finds patterns in data without labels

- No “correct answer” is provided

Example: Soil Type Clustering

- Features only: pH, organic matter, texture
- Model groups similar soils automatically — no target column
- The goal is to discover hidden structures or groupings

DART
DIGITAL AGRONOMY RESEARCH TEAM

Artificial Neural Networks: Introduction

History of ANNs:

- **1943:** McCulloch & Pitts proposed the first neural model using logic-based neurons

- **2010s:** Deep learning resurgence with big data, GPUs, and better algorithms

ELSEVIER

Neural Networks
Volume 2, Issue 5, 1989, Pages 359-366

Original contribution

Multilayer feedforward networks are universal approximators

Kurt Hornik

Technische Universität Wien Austria

Maxwell Stinchcombe, Halbert White [1]

University of California, San Diego USA

Received 16 September 1988, Accepted 9 March 1989, Available online 19 March 2003.

What do these dates mean?

Show less

Add to Mendeley Share Cite

https://doi.org/10.1016/0893-6080(89)90020-8

Get rights and content

Abstract

This paper rigorously establishes that standard multilayer feedforward networks with as few as one hidden layer using arbitrary squashing functions are capable of approximating any Borel measurable function from one finite dimensional space to another to any desired degree of accuracy, provided sufficiently many hidden units are available. In this sense, multilayer feedforward networks are a class of universal approximators.

Artificial Neural Networks: Introduction

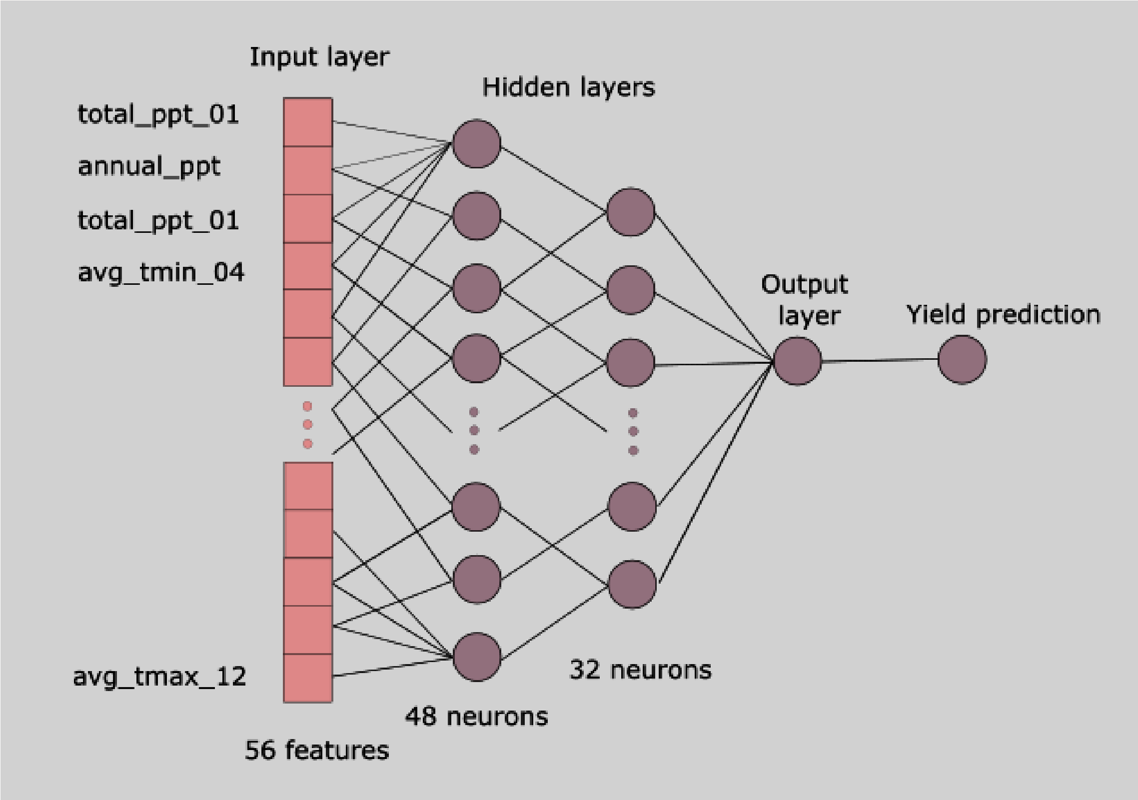


Fig. Architecture of ANNs

DART
DIGITAL AGRONOMY RESEARCH TEAM

ANNs: Analogy with linear regression

Linear regression:

$$y = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + b$$

$$y = \mathbf{w}^\top \mathbf{x} + b$$

x_i : Input features (e.g., rainfall, temperature, NDVI)
w_i : Coefficients (importance of each input)
b: Bias (baseline yield)
y: Output (e.g., crop yield)

ANNs:

$$\mathbf{y} = \phi\left(\mathbf{W}\mathbf{x} + \mathbf{b}\right)$$

x : Input features (e.g., rainfall, temperature, NDVI)
Φ : Activation function (e.g., ReLU)
W : Weights (different than coefficients in linear regression)
b: Bias
y: Output (e.g., crop yield)

DART DIGITAL AGRONOMY RESEARCH TEAM

ANNs: Activation functions

Why? Introduce non-linearity to model complex relationships

Sigmoid: $$\sigma(z) = \frac{1}{1 + e^{-z}}$$

$$\mathrm{ReLU}(z) = \max(0, z)$$

How to choose?

- For last layer: Based on the target variable
- For other layers: No specific rule, various combinations are tested

Reading material: Activation functions in Neural Networks – GeeksforGeeks

ANNs: Activation functions

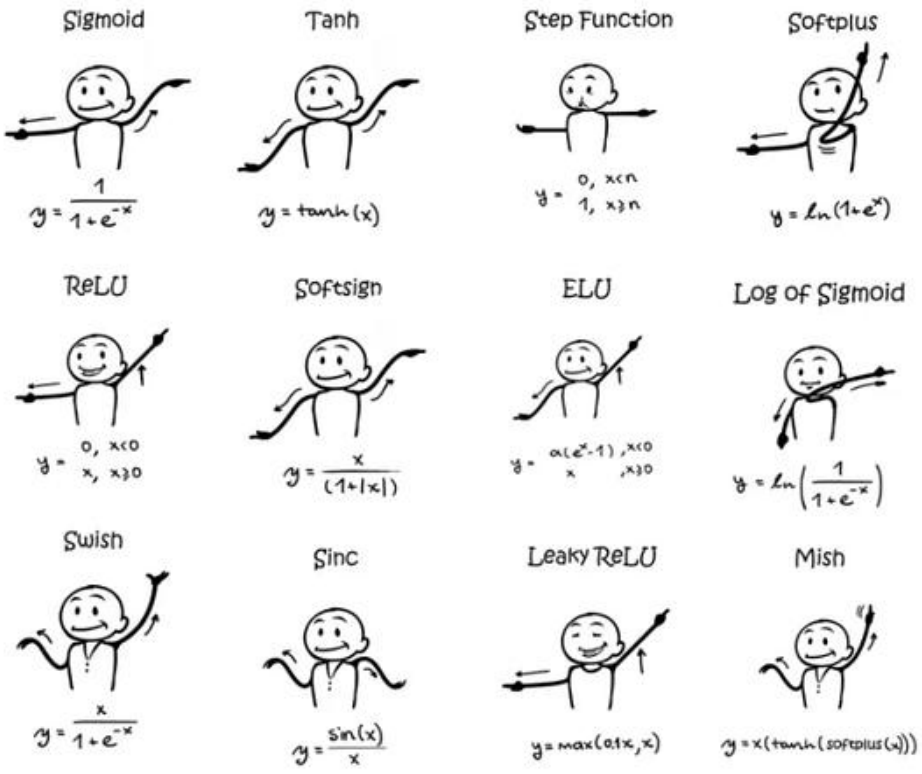


Fig. Activation functions.

[Ref: Activation Functions in Neural Networks | Shubhayu Majumdar | Medium]

DART
DIGITAL AGRONOMY RESEARCH TEAM

ANNs: Output calculation

Calculate the output for the given neural network

- Architecture: 2 features

Weights: [0.6, -0.4]
Bias: 0.2
Activation Function: ReLU

- Input Features:

x=[2 3] (row vector)

DART
DIGITAL AGRONOMY RESEARCH TEAM

ANNs: Output calculation

Calculate the output for the given neural network

- Architecture: 2 features

Layer 1 Weights:

node 1 : [0.5, -0.5]

node 2 : [0.2, 0.4]

Layer 2 Weights:

[0.3, 0.7]

Activation Function: ReLU

- Input Features :

x = [0.6 0.4] (row vector)

ANNs: Model training

- Features and corresponding targets are needed for model training
- Loss Function: Measuring Error: how far its prediction is from the actual value

Mean Squared Error (MSE): $Loss = \sum(y_{true} - y_{pred})^2$

Gradient Descent: Reducing the Error

- Backpropagation: Learning Internally
- Calculates how much each weight contributed to the error
- Weights are then updated to minimize the error
- This process is repeated across many iterations (epochs)

DART
DIGITAL AGRONOMY RESEARCH TEAM

ANNs: Building ANN model

What we choose:

- Input features, number of layers and neurons, activation functions, epochs

What the model learns automatically:

- Weights and function

Demo: A Neural Network Playground

DART
DIGITAL AGRONOMY
RESEARCH TEAM

Python code

https://tinyurl.com/unicampcolab

DART
DIGITAL AGRONOMY
RESEARCH TEAM

Introduction to the Dataset

Brief overview of the data and data sources

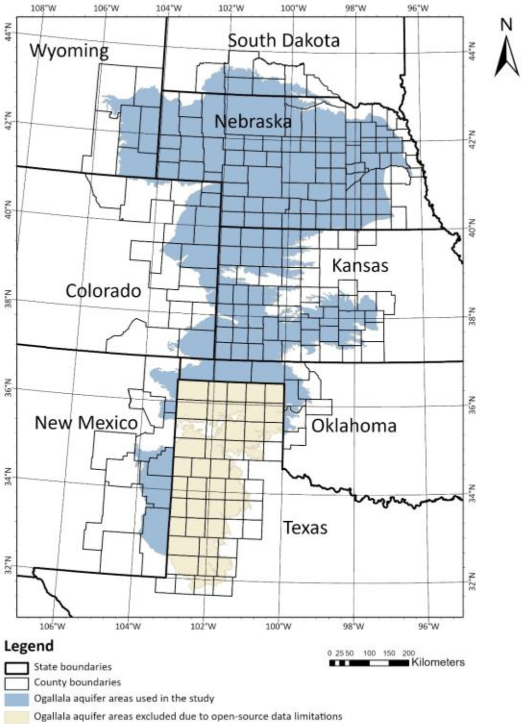


Fig. Ogallala aquifer (the largest underground water reserve in North America)

Fig. Alfalfa forage crop (the most preferable forage with high nutritional value for dairy cattle)

DART DIGITAL AGRONOMY RESEARCH TEAM

KANSAS STATE UNIVERSITY

Brief overview of the data and data sources

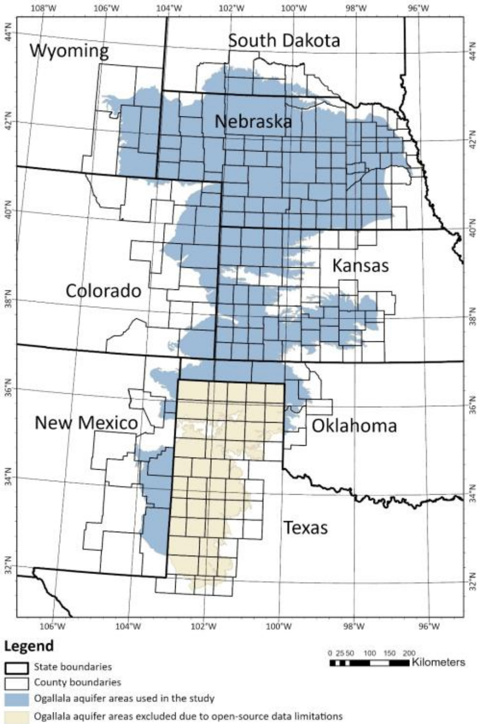


Fig. Ogallala aquifer (the largest underground water reserve in North America)

PRISM CLIMATE GROUP — Climate data

USDA Natural Resources Conservation Service, United States Department of Agriculture — Soil data

USDA NASS — Alfalfa yield data in tons/ha

DART DIGITAL AGRONOMY RESEARCH TEAM

Climate and Soil features

Features list	Acronym	Unit
Accumulated Growing Degree Days	GDD	ºC day
Monthly total precipitation	total_ppt_*	mm
Annual total precipitation	annual_ppt	mm
Number of no precipitation days	noppt_*	unitless
Annual number of no precipitation days	annual_noppt	unitless
Average monthly minimum temperature	avg_tmin_*	ºC
Average monthly maximum temperature	avg_max_*	ºC
Monthly mean temperature	avg_tmean_*	ºC
Monthly mean dew point temperature	avg_tdmean_*	ºC
Average monthly minimum vapor pressure deficit	avg_vpdmin_*	hPa
Average monthly maximum vapor pressure deficit	avg_vpdmax_*	hPa
Sand	-	%
Silt	-	%
Clay	-	%
Organic matter	OM	%
Bulk density	BD	g/cm^3

* Can vary from 1 to 12, referring to January to December.

Precipitation

Temperature

Vapor pressure deficit

Soil texture

DART DIGITAL AGRONOMY RESEARCH TEAM

SHAP for the model interpretability

Explainable ML matters in Agriculture

- Increasing adoption of Machine Learning in precision agriculture (yield prediction, irrigation scheduling, disease detection)
- Need for trust and transparency in decision-making
- SHAP (SHapley Additive exPlanations) values = interpretable machine learning

- SHAP values can help to explain **individual predictions**
- Based on **Shapley values** from cooperative game theory
- Each feature contributes to the final prediction—SHAP tells us *how much*

DART
DIGITAL AGRONOMY
RESEARCH TEAM

SHAP: Cooperative Game Theory

- Developed by Lloyd Shapley in 1953
- It is a mathematical framework where players work together to achieve a total reward (payout).
- **Goal**: Fairly distribute the total gain among the players based on their contributions.

Agricultural Analogy:

Imagine different **features** (e.g., precipitation, temperature, soil texture) are like **players in a team** that collectively influence **crop yield**.

- Question: *How much did each "player" contribute to the final yield prediction?*

DART DIGITAL AGRONOMY RESEARCH TEAM

SHAP: Fair Contribution of Each Feature

- **Shapley value =** Average contribution of a feature across all possible combinations of features.

Weighting factor

Marginal contribution

$$\phi_i = \sum_{S \subseteq N \setminus \{i\}} \frac{|S|!\,(|N| - |S| - 1)!}{|N|!} [(v(S \cup \{i\}) - v(S)]$$

Where:

- ϕ_i : Shapley value (fair contribution) for feature *i* to the prediction
- *S*: A subset of features excluding *i*
- *v(S)*: The model prediction using features in set *S*
- *N*: Total set of features (e.g., precipitation, temperature, soil texture)

DART DIGITAL AGRONOMY RESEARCH TEAM

SHAP: Summary Plot

Let's make a **summary plot** with the dataset provided to achieve the **global view** of feature importance across the entire dataset

DART
DIGITAL AGRONOMY
RESEARCH TEAM

SHAP: Force Plot

Let's make a **force plot** with the dataset provided to achieve the **local explanation** for a single prediction in the dataset

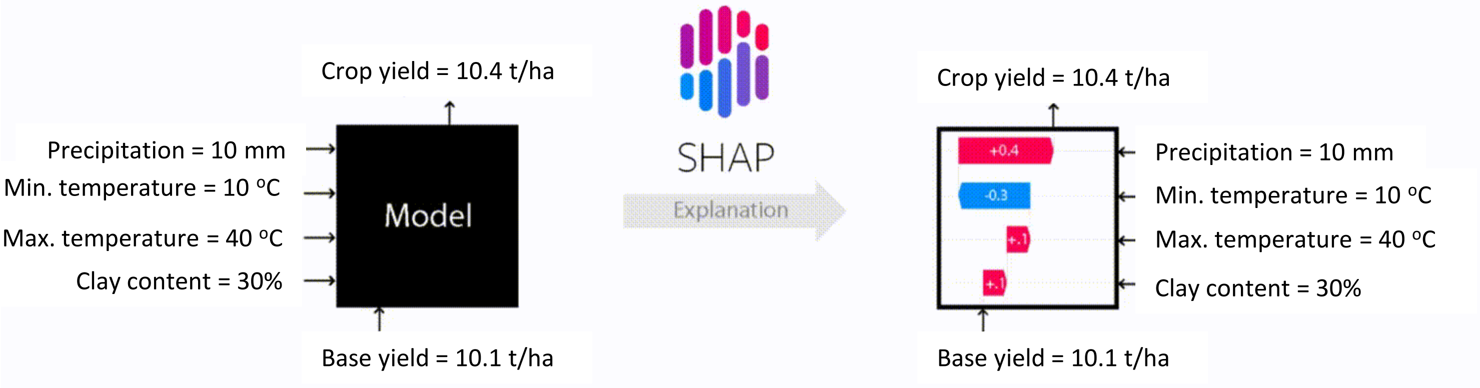
Base value: The **average model output** over the training data. It's the starting point before any features are considered.

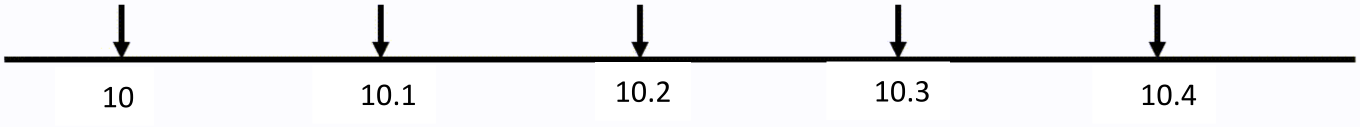
Final prediction for a specific instance: $f(x) = \textit{base value} + \sum_{i=1}^{n} \phi_i$

Force plot shows how each feature pushed the prediction higher or lower compared to the base value.

DART
DIGITAL AGRONOMY RESEARCH TEAM

SHAP: Calculation Demonstration





x_1: Precipitation

x_2: Min. temp.

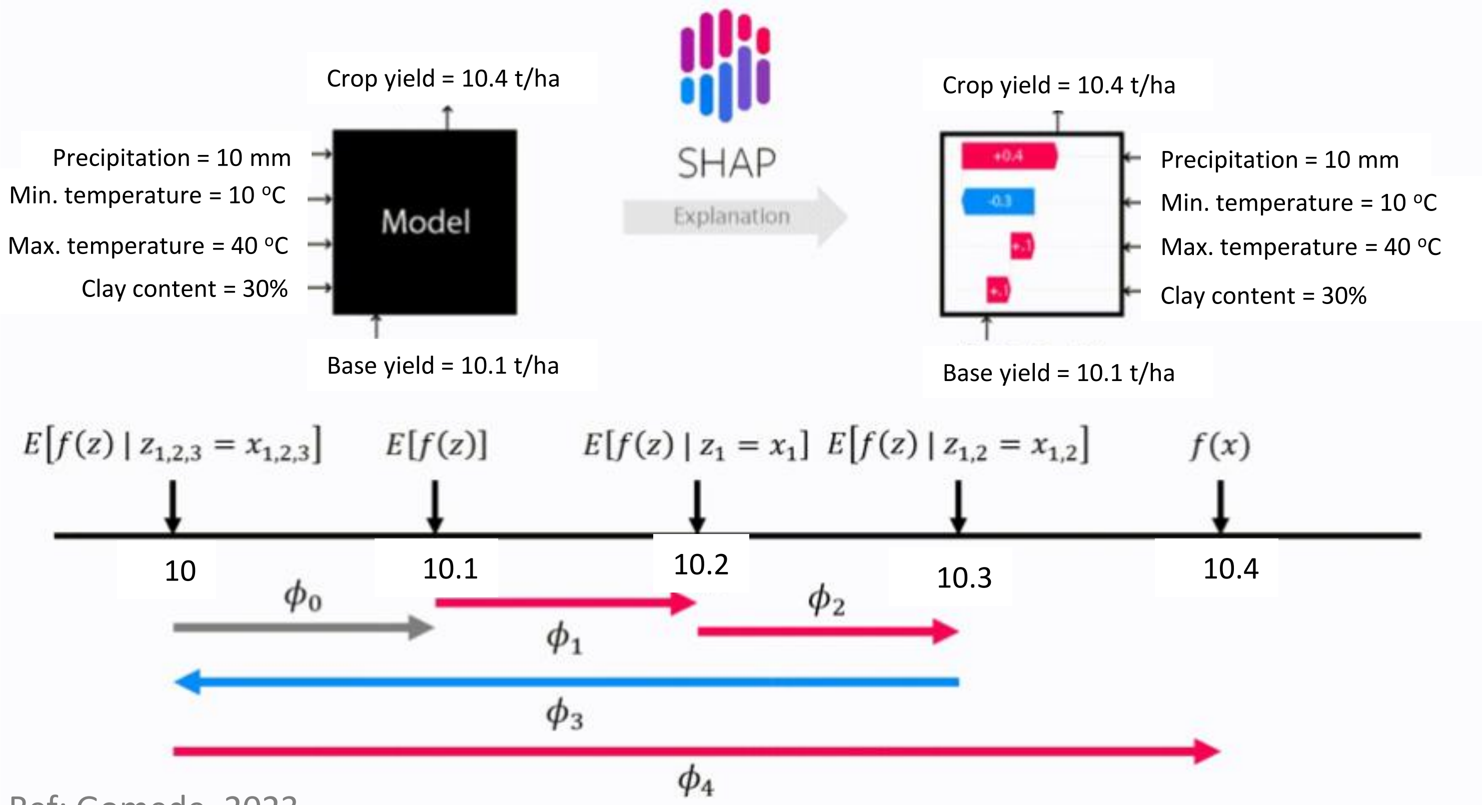
x_3: Max. temp.

x_4: Clay content

Ref: Gomede, 2023

DART DIGITAL AGRONOMY RESEARCH TEAM

SHAP: Calculation Demonstration



x_1: Precipitation

x_2: Min. temp.

x_3: Max. temp.

x_4: Clay content

Ref: Gomede, 2023

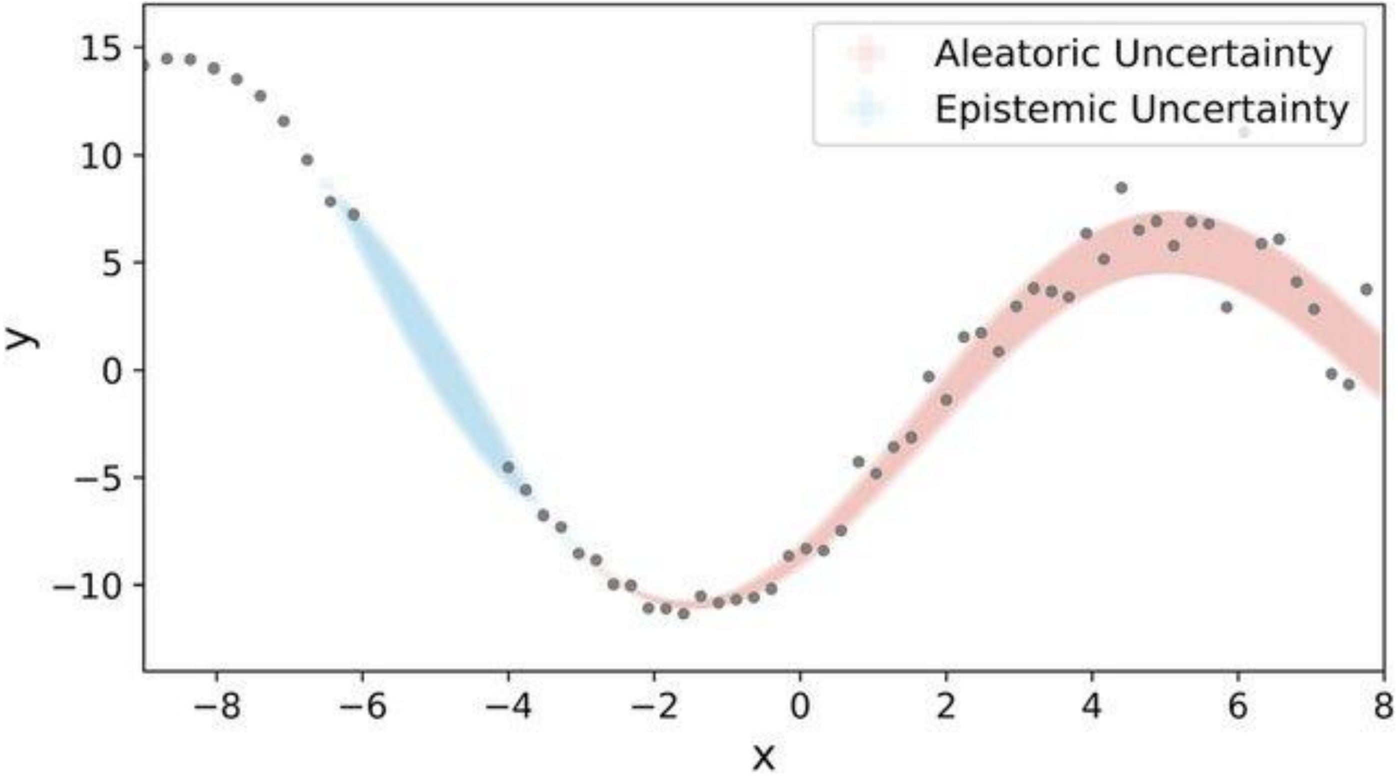
DART DIGITAL AGRONOMY RESEARCH TEAM

SHAP: Waterfall Plot

Let’s make a **waterfall plot** with the dataset provided to achieve the **local explanation** for a single prediction in the dataset

End of SHAP for the model interpretation

Aleatoric and epistemic Uncertainty



Ref: (PDF) Explainable uncertainty quantifications for deep learning-based molecular property prediction

Aleatoric and epistemic Uncertainty

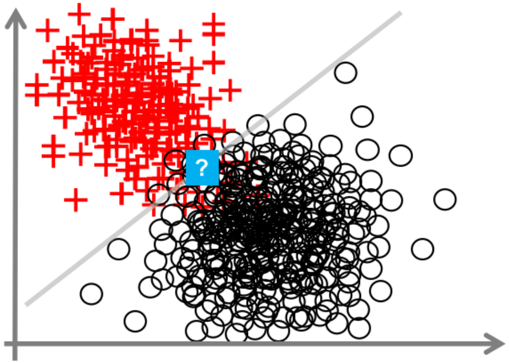


***Fig** – Aleatoric uncertainty*

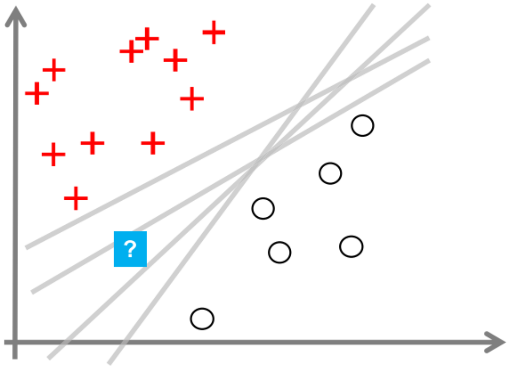


***Fig** – Epistemic uncertainty*

Uncertainty type	Aleatoric	Epistemic
Arises from	Inherent randomness in data	Limited understanding of process
May reduce with more	Features	Data
Modelled as	Probability distributions for outcomes	Probability distribution for parameters
Also known as	Model uncertainty	Parameter uncertainty

Bayesian Neural Network: BNN

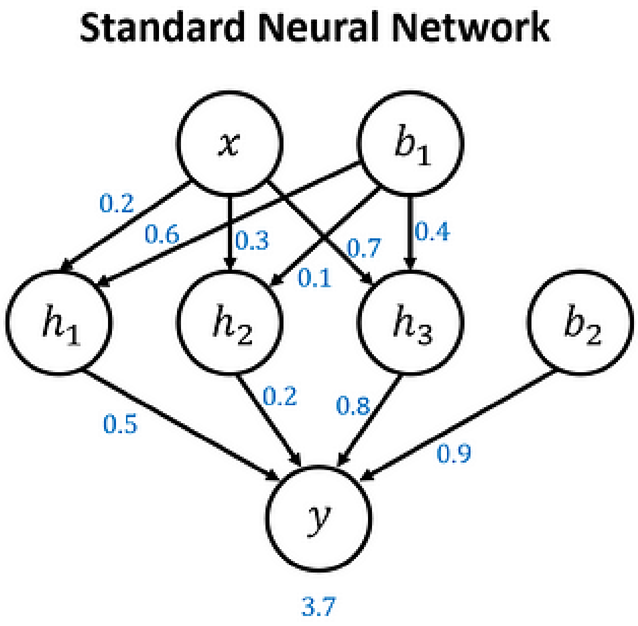


Fig. Conventional ANN

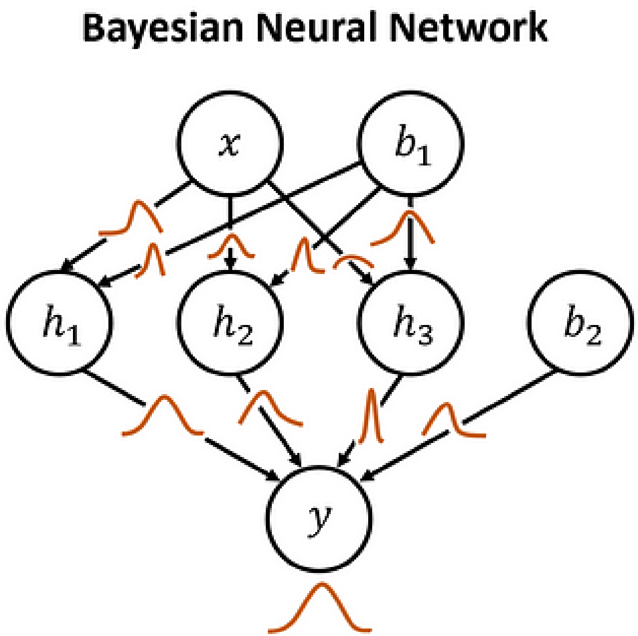


Fig. Bayesian ANN

Ref: Why You Should Use Bayesian Neural Network | by Yeung WONG | Towards Data Science

BNN: Architecture

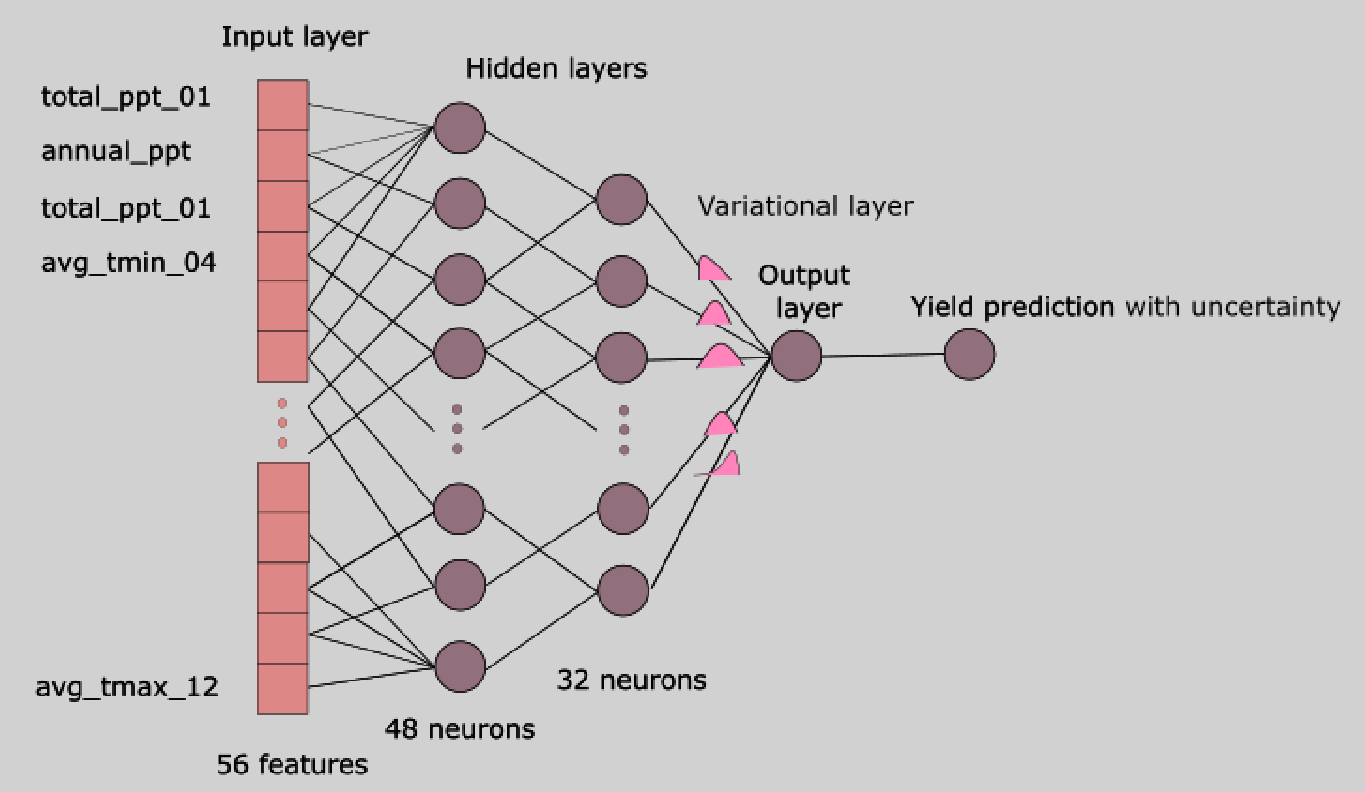


Fig. Bayesian Neural Network Architecture

Lessons learned

Bayesian Neural Networks: Making ANNs *Uncertainty Aware*

- You want to predict outcomes with uncertainty (e.g., yield prediction, rainfall, evapotranspiration).
- Data is limited, noisy, or incomplete.
- Decision-making depends on confidence in predictions (e.g., irrigation planning, crop insurance, early warnings).

SHAP: Making ANNs *Interpretable*

- You want to understand why the model made a prediction.
- Stakeholders need transparent decision support.
- For feature importance analysis.

Post-workshop assessment

https://tinyurl.com/mlunicamp2025

Questions?

Contact:

Prasad Deshpande (Post doc) deshpande@ksu.edu
Sourajit Dey (PhD student) sdey@ksu.edu

Follow us: DART DIGITAL AGRONOMY RESEARCH TEAM

LinkedIn: K-State-Digital Agronomy Research Team
Instagram: ksu_digitalagronomy

Kansas State University