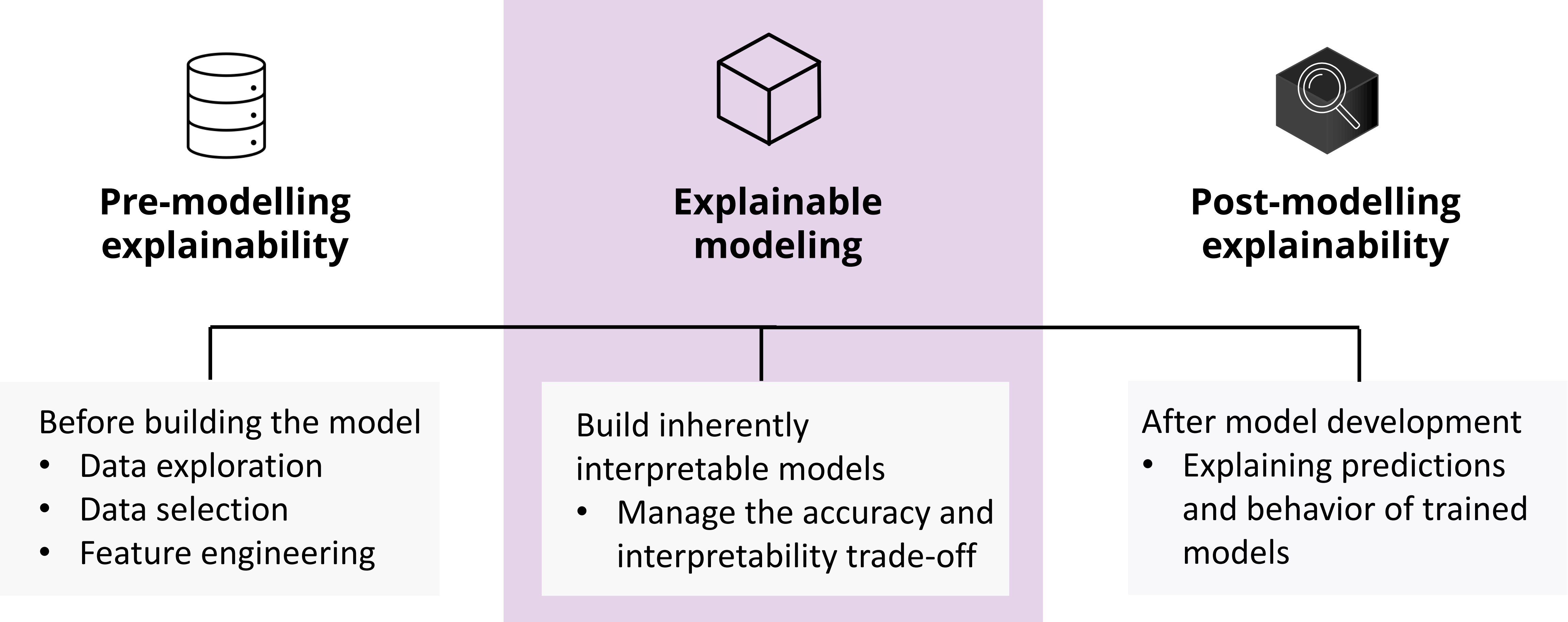
# In-modeling Explainability

Explainable and Trustworthy AI

Eliana Pastor

# Stages of Explainability

Explainability involves the entire AI development pipeline



**Pre-modelling explainability**

Before building the model
- Data exploration
- Data selection
- Feature engineering

**Explainable modeling**

Build inherently interpretable models
- Manage the accuracy and interpretability trade-off

**Post-modelling explainability**

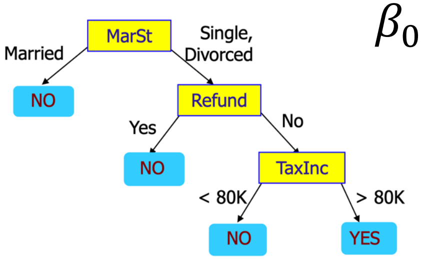
After model development
- Explaining predictions and behavior of trained models

# Stages of Explainability – Explainable modelling

Design, train and adopt more interpretable/explainable models

- Adopting **an inherently explainable models**
    - does not automatically guarantee explainability (e.g., deep trees, linear models on high dimensional data)
    - Problem of explainability vs performance trade-off: interpretable models are typically less performing

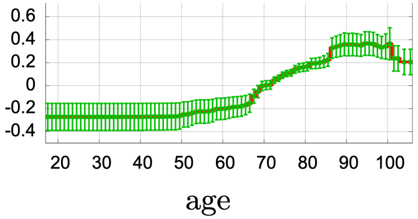
**Trees**



**Linear models**

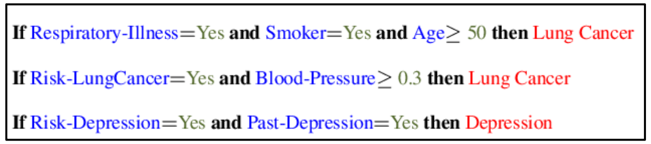
$$\beta_0 + \sum_i \beta_i x_i$$

**GAMs, GA²Ms, GLMs**



Caruana et al. "Intelligible Models for HealthCare: Predicting Pneumonia Risk and Hospital 30-day Readmission." KDD 2015

**Decision sets - Rules**



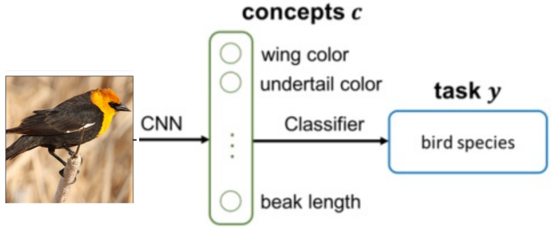
**If** Respiratory-Illness=Yes **and** Smoker=Yes **and** Age$\geq$ 50 **then** Lung Cancer

**If** Risk-LungCancer=Yes **and** Blood-Pressure$\geq$ 0.3 **then** Lung Cancer

**If** Risk-Depression=Yes **and** Past-Depression=Yes **then** Depression

Lakkaraju et al. "Interpretable decision sets: A joint framework for description and prediction." KDD 2016

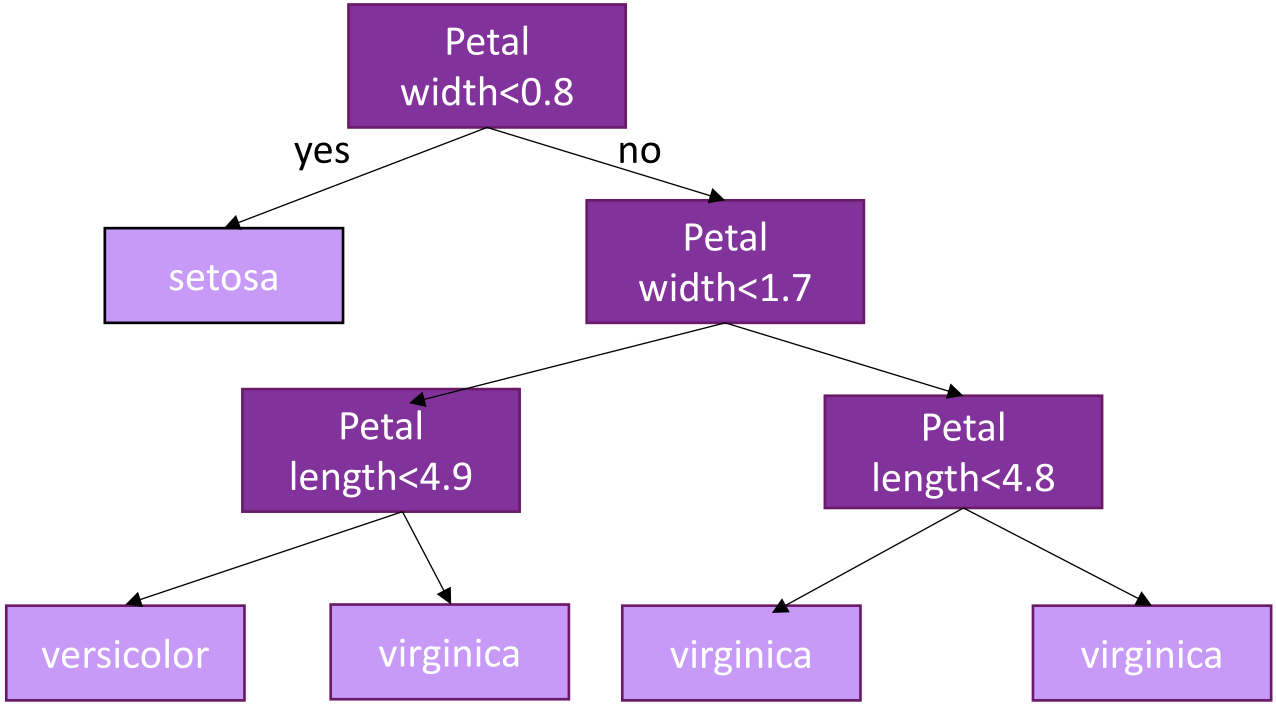
**Concept-based models**



Koh, Pang Wei, et al. "Concept bottleneck models." ICML 2020.

# Decision trees

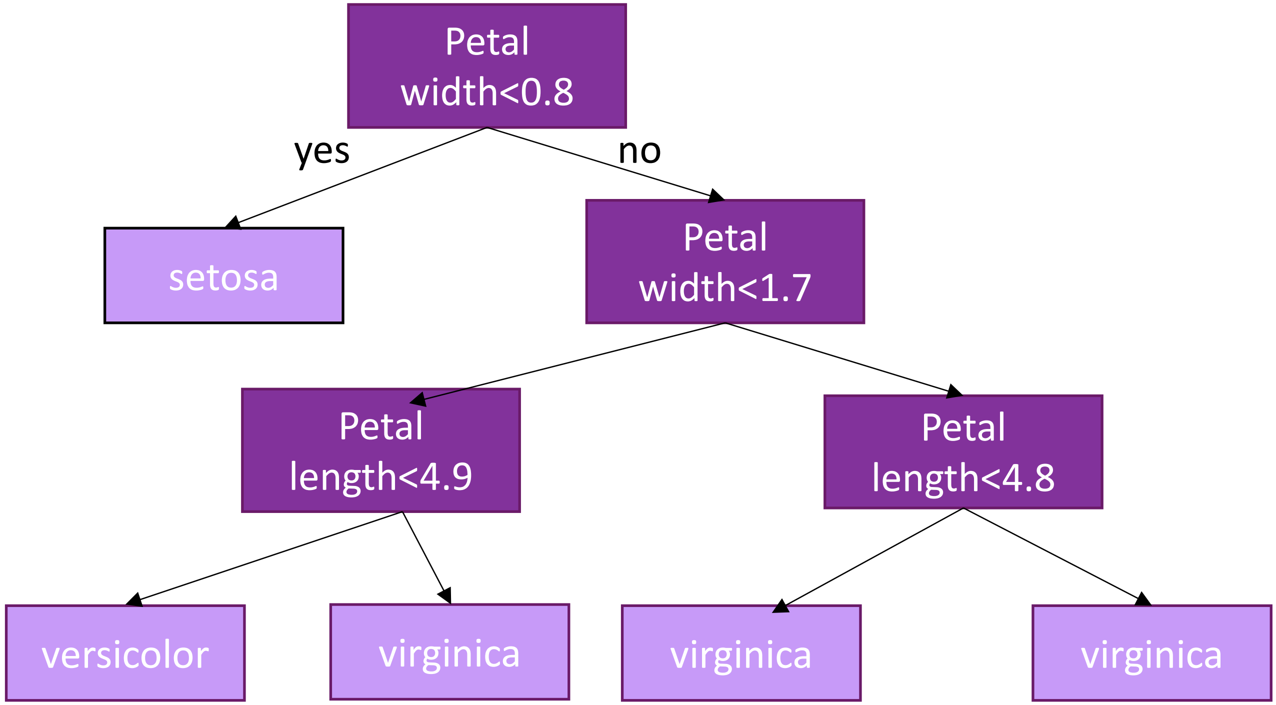
- Simple supervised models used for both classification and regression tasks.
- **Tree-like structure**
- Each **internal** node represents a decision based on a feature
- Each **leaf** node represents the outcome or the decision



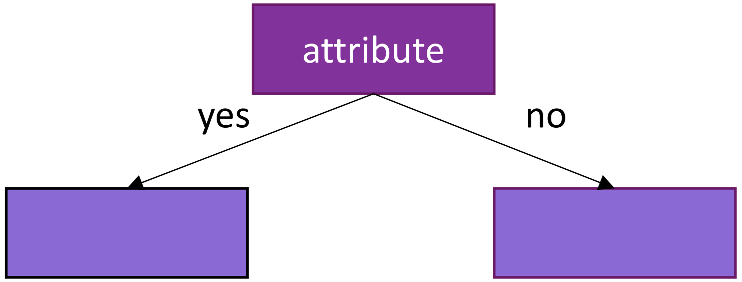
# Structure - Decision trees

**Structure**

- Root Node: topmost node where the first decision is made
- Decision or Inner Nodes: Nodes that represent decisions or tests on attribute
- Edges: possible outcomes of a decision
- Leaf Nodes: terminal nodes that provide the final decision



# Building a Decision Tree



1. Begin with the entire dataset at the root node

2. Select best splitting attribute and value based on a splitting criterion (e.g., Gini Impurity).

3. Partition the dataset into subsets based on the values of the selected attribute.

4. Recursively apply steps 2 and 3 to each subset until one of the following conditions is met:
   - All instances in the subset belong to the same class.
   - No more attributes to split on.
   - Stopping criteria (e.g., maximum depth, minimum leaf samples per leaf) are met.

5. Assign a class label to each leaf node based on the majority

# Decision trees interpretability

- Decision trees offer both
  - Global interpretability
  - Local interpretability

# Global interpretability for Decision trees

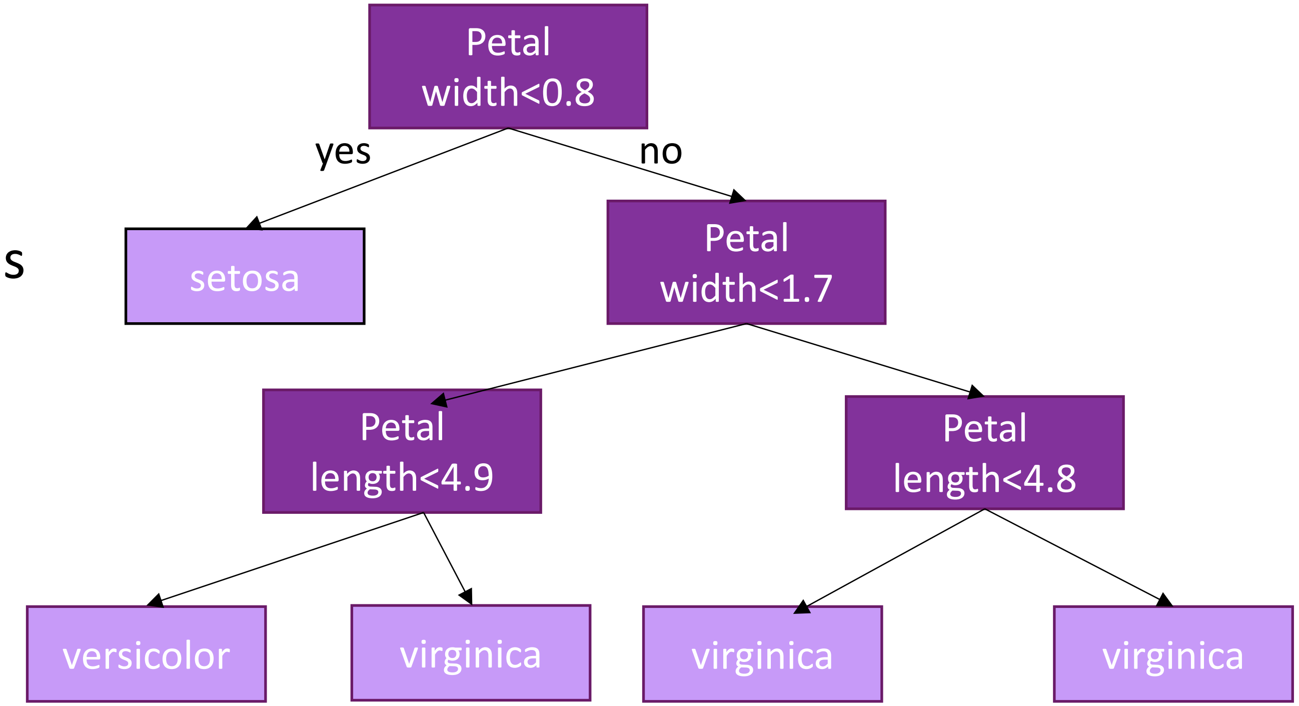
Global interpretability focuses on understanding the overall behavior and workings of the model across the entire dataset.

- Tree Structure
- Decision rules from the tree
- Feature Importance

# Global interpretability for Decision trees

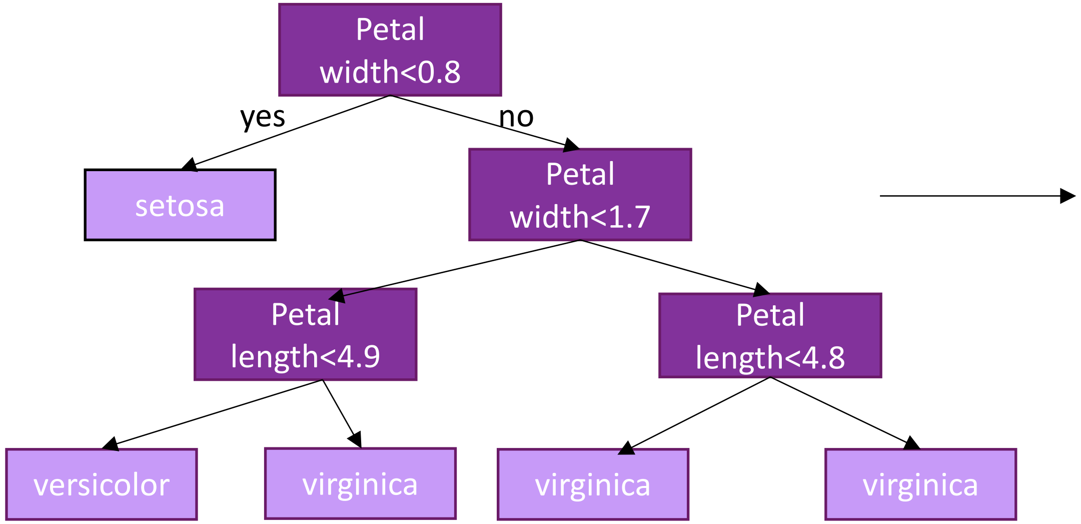
**Tree structure**

Analyze the decision paths of the tree models



# Global interpretability for Decision trees

## Decision rules from the tree

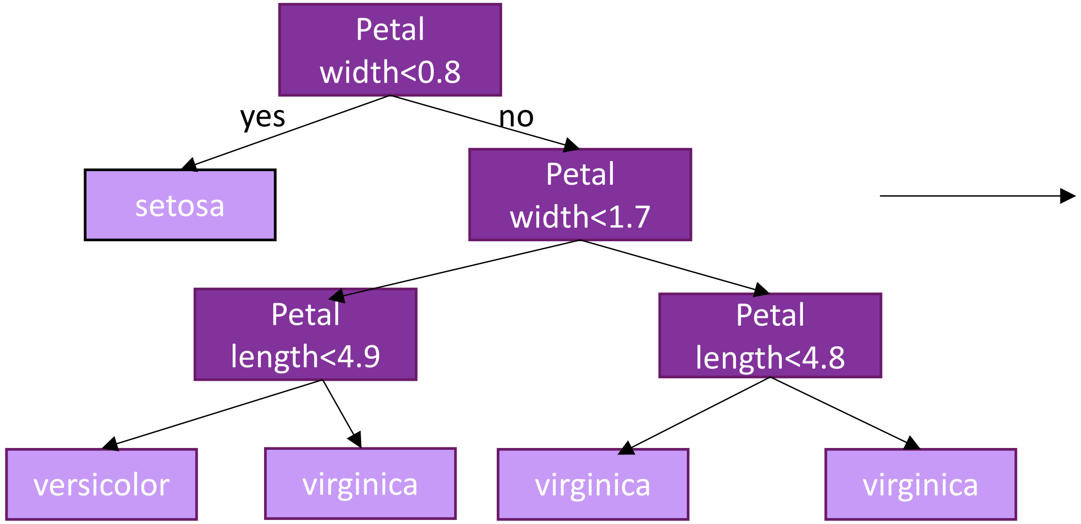


width<0.9 → setosa
width in [0.8, 1.7], length<4.9 → versicolor
width in [0.8, 1.7], length>4.9 → virginica
width > 1.7], length>4.9 → virginica

For some users, rules are more easy to understand

# Global interpretability for Decision trees

## Feature Importance



Petal width<0.8

yes

no

setosa

Petal width<1.7

Petal length<4.9

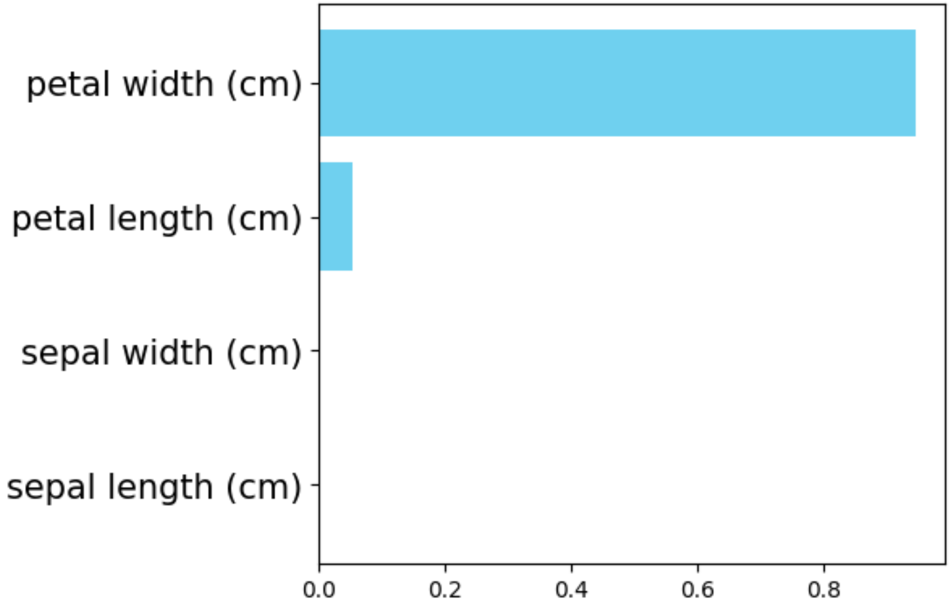
Petal length<4.8

versicolor

virginica

virginica

virginica



# Feature Importance for Decision Trees

Multiple ways to compute the feature importance

- **Impurity-based feature importance**
  - The importance of a feature is the (normalized) total reduction of the impurity criterion obtained by using that feature for splitting
    - Also known as GINI importance

- **Depth-based Importance**
  - Higher importance to features that appear closer to the root node

- **Path-based Importance**
  - Features that appear more frequently in the tree have higher important

# Impurity-based feature importance

Based on the notion of impurity, e.g., Gini Index

t | # Class 1: 10<br># Class 2: 10 | GINI = 0.5

Gini Index for a given node t:

t | # Class 1: 20<br># Class 2: 0 | GINI = 0

$$GINI(t) = 1 - \sum_{j} [p(j|t)]{}^\wedge 2$$

where $p(j|t)$ is the relative frequency of class j at node t

- Maximum (1 - 1/nc ) when each class occurs with equal probability, implying higher impurity degree
- Minimum (0.0) when all instances belong to one class, implying lower impurity degree

# Impurity-based feature importance

The importance of a feature is computed as the (normalized) total reduction of the impurity criterion obtained by using that feature for splitting.

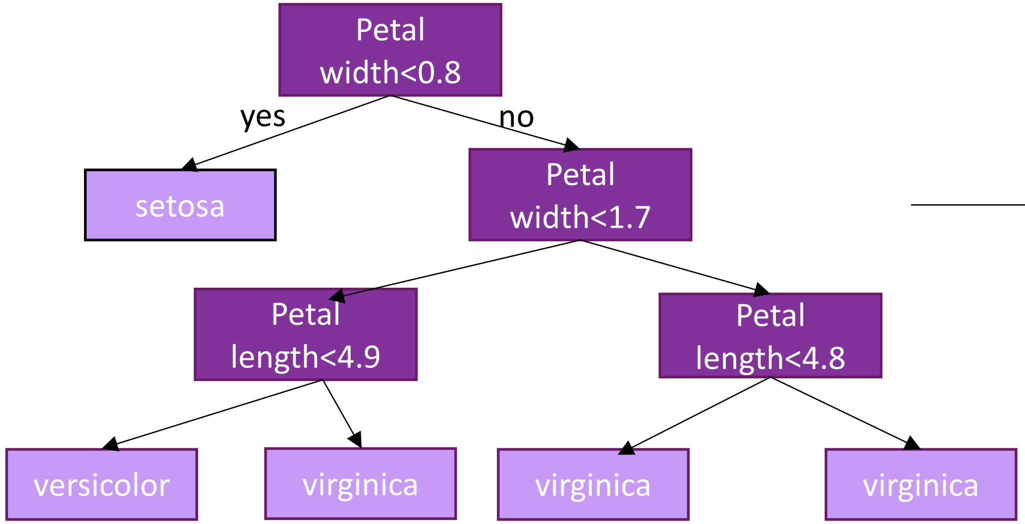
**Computation**

- For each split, measure how much it has reduced the impurity (e.g., Gini index) compared to the parent node
    - Difference in impurity between the parent node and its child nodes
    - Weight the difference by the number of samples in each node
    - Increment the total importance of the attribute used for the splitting by this importance
- Scale the sum of all importance in the scale 0-1
- Each feature importance indicates its relevance to overall model importance.

# Impurity-based feature importance

**Global interpretability**

Global importance of each attribute



Petal width<0.8

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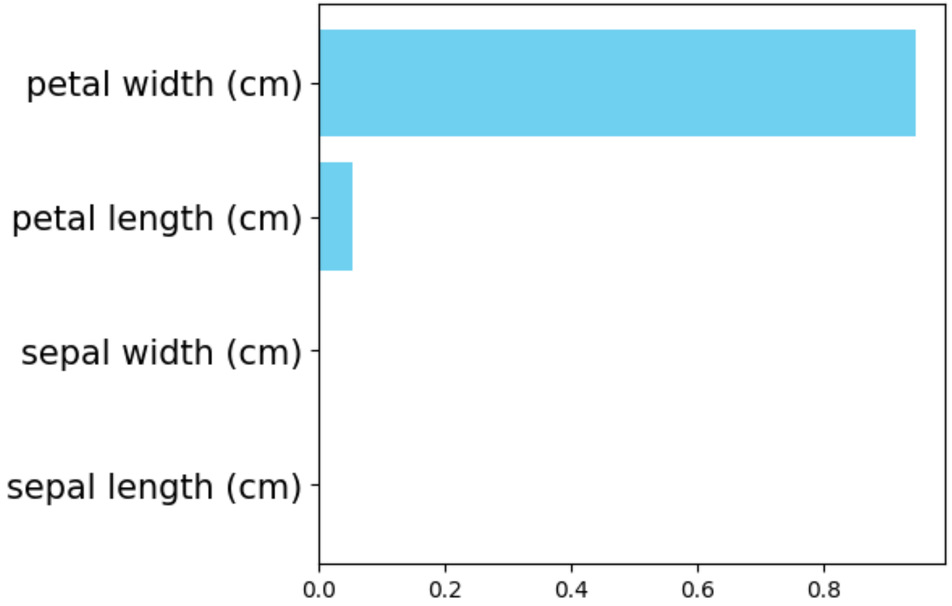
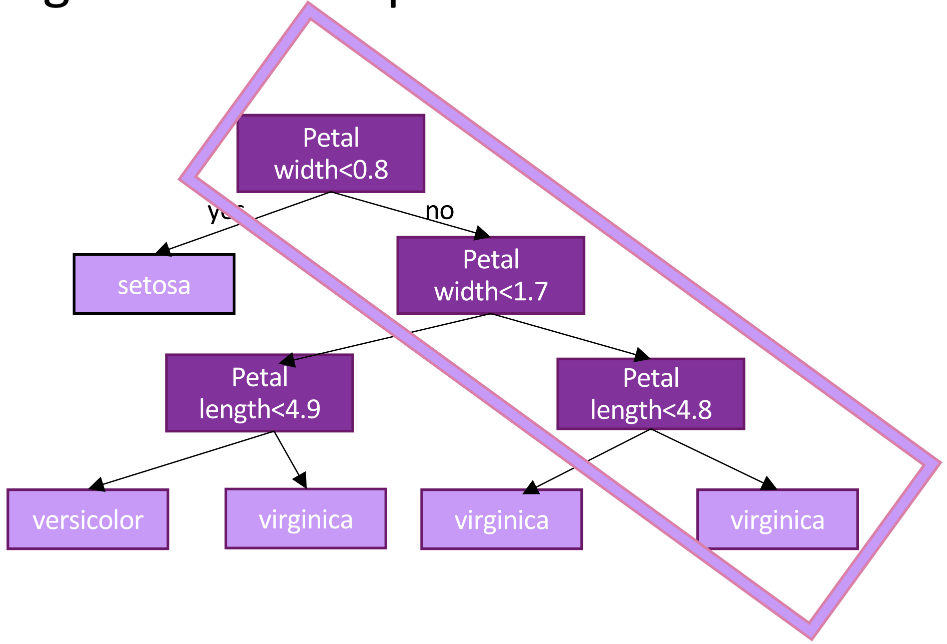


# Local interpretability for Decision trees

Local interpretability refers to understanding the behavior and predictions of the model for individual instances.

It explain why a particular prediction is made for a specific input.

- **Path Explanation**: tracing the decision path from the root node to the leaf node for an instance



# Local interpretability for Decision trees

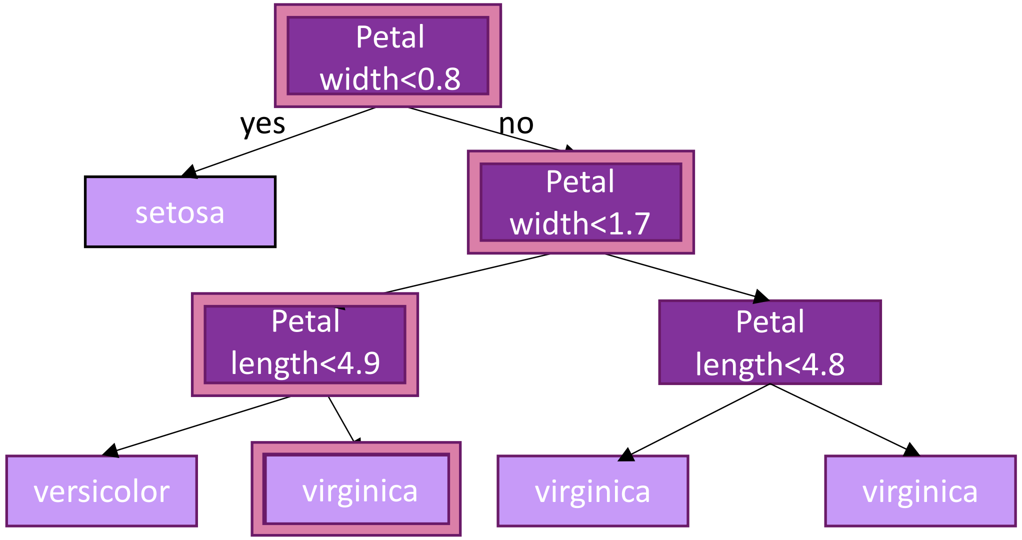
**Example**

**Instance**

Petal width = 1.1, petal length=5, sepal width = 1, sepal lenght=1

**Decision Path**

Petal width<0.8 = False, petal width <1.7 = True, Petal legth < 4.9 = False



# Advantages of Trees

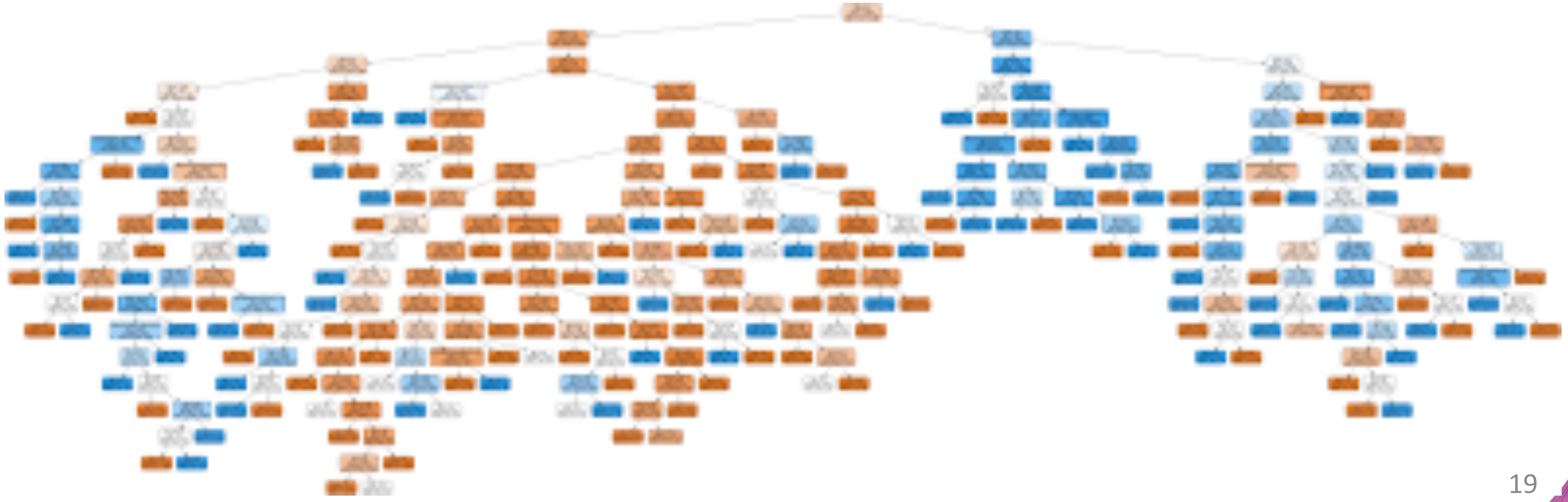
- Offer multiple insights
    - Global interpretability
    - Local interpretability
    - + Subgroup. Each path actually covers a subset of the data. Easier to understand than individual points

- (Generally) Easy to interpret, also globally
    - Human-friendly explanations, the interpretation is simple
- Tree structures offers a build-in visualization, enhance understanding
- Facilitates communication with non-technical stakeholders
- Being interpretable, users can assess if they can trust the model

# Limitations of Trees

- Low accuracy compared to more complex model
  - Interpretability accuracy trade-off

- Decision trees are very interpretable – if they are small!
  - Few splitting nodes
  - Low depth



# Decision rules

Classify instances by using “if…then…” rules

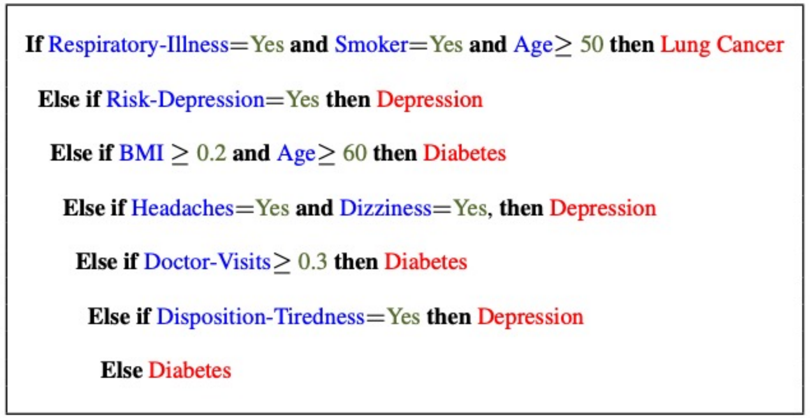
- **Rule: (Condition) → y** where
  - Condition is a conjunction of simple predicates
  - y is the class label

- Rule extraction
  - Rule Induction Algorithms
    - e.g., CN2 or RIPPER, explicitly generate rules from the training data based
  - Associative classifiers
  - From decision trees

# Decision rules

- **Decision list**
    - Ordered decision rules
    - Prediction based on the first rule satisfying the instance

- **Decision set**
    - Independent rules
    - Rules are mutually exclusive, or there is a strategy for resolving conflicts, such as majority voting



**If** Respiratory-Illness=Yes **and** Smoker=Yes **and** Age≥ 50 **then** Lung Cancer

**Else if** Risk-Depression=Yes **then** Depression

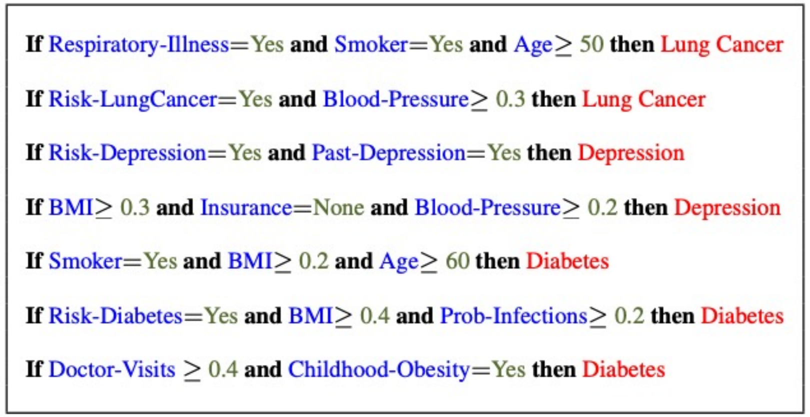
**Else if** BMI ≥ 0.2 **and** Age≥ 60 **then** Diabetes

**Else if** Headaches=Yes **and** Dizziness=Yes, **then** Depression

**Else if** Doctor-Visits≥ 0.3 **then** Diabetes

**Else if** Disposition-Tiredness=Yes **then** Depression

**Else** Diabetes



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**If** Risk-LungCancer=Yes **and** Blood-Pressure≥ 0.3 **then** Lung Cancer

**If** Risk-Depression=Yes **and** Past-Depression=Yes **then** Depression

**If** BMI≥ 0.3 **and** Insurance=None **and** Blood-Pressure≥ 0.2 **then** Depression

**If** Smoker=Yes **and** BMI≥ 0.2 **and** Age≥ 60 **then** Diabetes

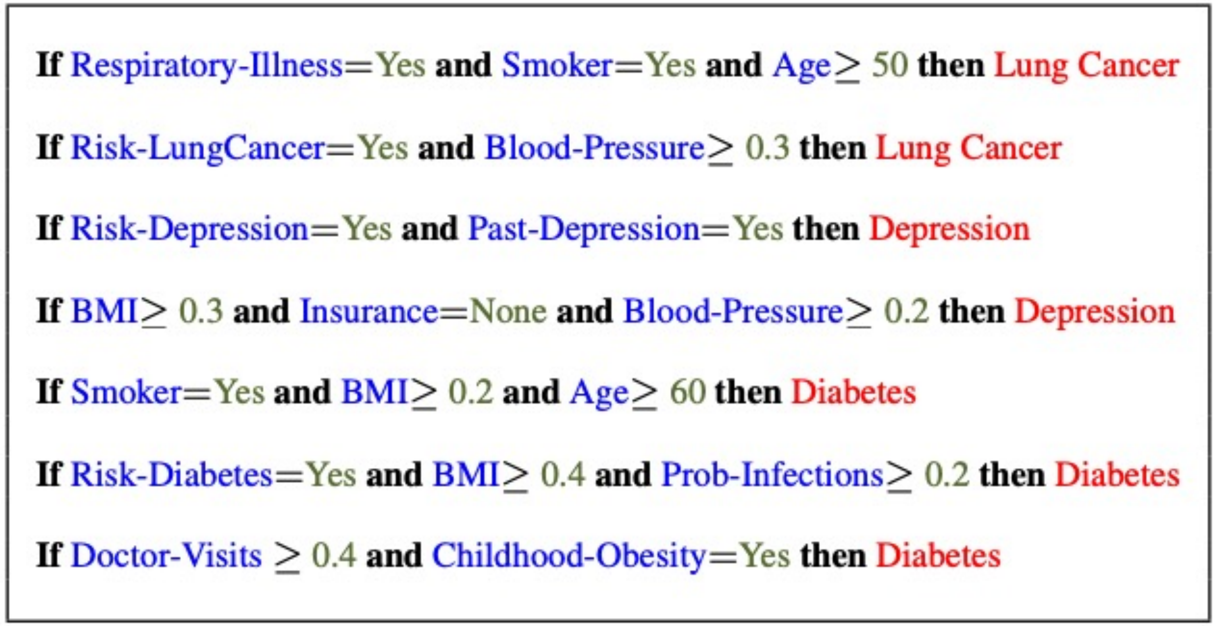
**If** Risk-Diabetes=Yes **and** BMI≥ 0.4 **and** Prob-Infections≥ 0.2 **then** Diabetes

**If** Doctor-Visits ≥ 0.4 **and** Childhood-Obesity=Yes **then** Diabetes

Lakkaraju et al. "Interpretable decision sets: A joint framework for description and prediction." KDD 2016

# Global Interpretability for Decision rules

- Analyze rules themselves



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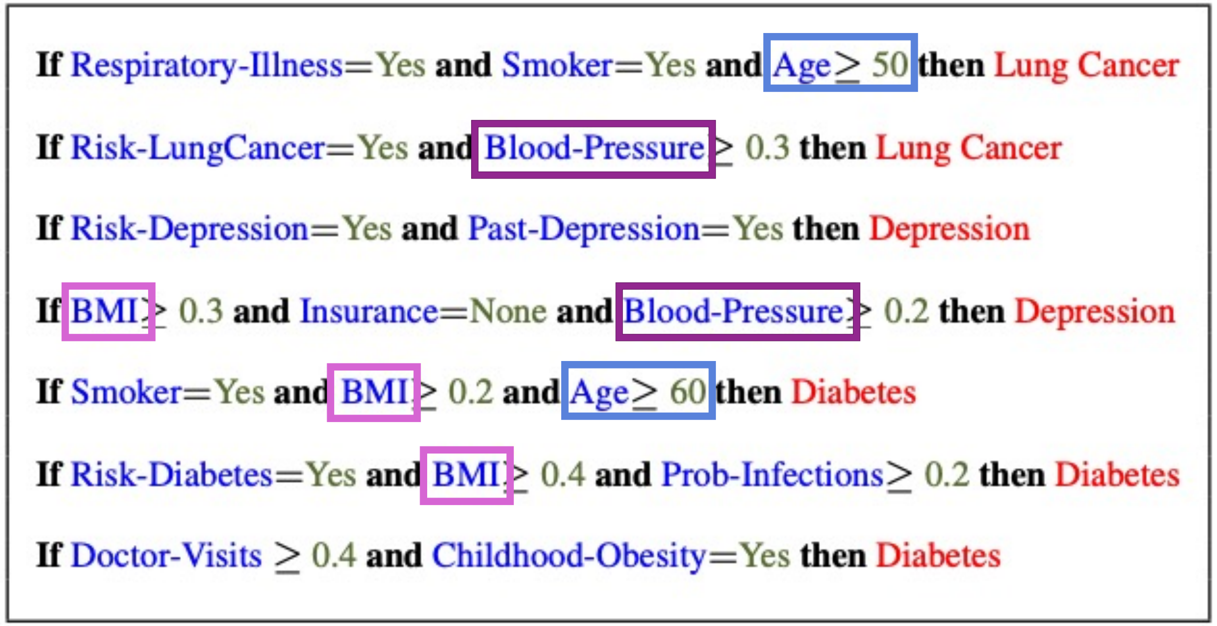
**If** Risk-Diabetes=Yes **and** BMI$\geq$ 0.4 **and** Prob-Infections$\geq$ 0.2 **then** Diabetes

**If** Doctor-Visits $\geq$ 0.4 **and** Childhood-Obesity=Yes **then** Diabetes

# Global Interpretability for Decision rules

- Feature importance
  - Features that appear in multiple decision rules are likely to be more important



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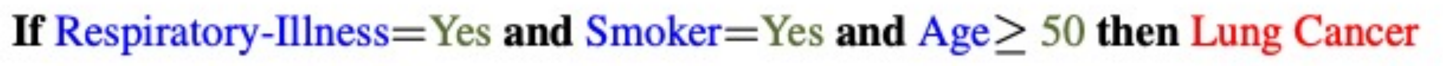
**If** Doctor-Visits $\geq$ 0.4 **and** Childhood-Obesity=Yes **then** Diabetes

# Local Interpretability for Decision rules

- Analyze individual rule satisfying the instance



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# Advantages of Rules

- Offer multiple insights
  - Global interpretability
  - Local interpretability
  - + Subgroup. Each rule actually covers a subset of the data

- (Generally) easy to interpret, also globally
  - Human-friendly explanations, the interpretation is simple
- Expressive as tree, but more compact
  - Some users find them **more interpretable than trees**
- Facilitates communication with non-technical stakeholders
- Being interpretable, users can assess if they can trust the model

# Limitations of Rules

- Often require categorical data
  - Numerical feature should be discretized

- Low accuracy compared to more complex model
  - Interpretability accuracy trade-off

- Rules are very interpretable – if they are compact!
  - Few rules
  - Short rules

# Linear regression

A linear regression model predicts the target as a weighted sum of the feature inputs.

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + .. + \beta_p x_p$$

**Interpret the Coefficients**

- The coefficients $\beta_i$ represents the change in the dependent variable for a one-unit change in the corresponding independent variable, holding all other variables constant.
  - i.e., Increasing $\mathrm{x}_i$ by one unit changes the estimated outcome by its $\beta_i$ .
    - If $\beta_i$ is positive, it indicates that as $\mathrm{x}_i$ increases, $y$ also increases.
    - If $\beta_i$ is negative, it indicates that as $\mathrm{x}_i$ increases, $y$ decreases.
- The intercept $\beta_i$ represents the value of the dependent variable when all independent variables are set to zero.
  - In some cases, the interpretation might not be meaningful, especially if zero doesn't have a practical meaning for the variables.

# Example - Interpreting Linear Regression

Goal. Predict the salaries of individuals based on their years of experience and level of education. We want to build a linear regression model to predict salaries based on these two variables.

Model.

$$Salary = \beta_0 + \beta_1 \times Years\ of\ Experience + \beta_1 \times Level\ of\ Education$$

$\beta_0$ = 40000, $\beta_1$ = 3000, $\beta_2$ = 2000

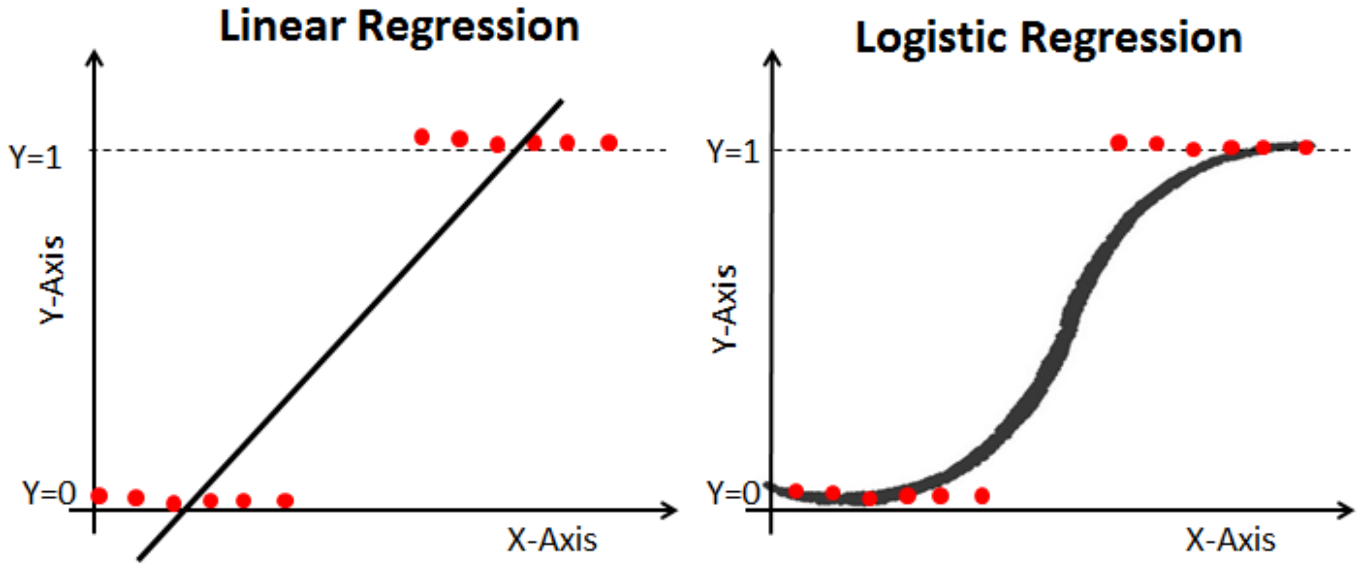
- Intercept : A person with zero years of experience and zero years of education would have a predicted salary of $40,000.
- For each additional year of experience, the predicted salary is expected to increase by $3000, holding the level of education constant.
- For each additional year of education, the predicted salary is expected to increase by $2000, holding years of experience constant.

# Inherently explainable models
# Logistic regression

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + .. + \beta_p x_p$$

$$\text{logistic}(x) = \frac{1}{1+\exp(-x)}$$

$$P(y = 1) = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 x_1 + \beta_2 x_2 + .. + \beta_p x_p))}$$



# Logistic regression

$$P(y=1) = \frac{1}{1+\exp(-(\beta_0+\beta_1 x_1\ +\beta_2 x_2 + .. + \beta_p x_p))}$$

**Log odds**

$$\ln\left(\frac{P(y=1)}{1-P(y=1)}\right) = \ln(Odds) = \beta_0+\beta_1 x_1\ +\beta_2 x_2 + .. + \beta_p x_p$$

- The coefficients represent the change in the log odds of the event occurring for a one-unit change in the corresponding predictor variable, holding all other variables constant.

# Logistic regression

$$\frac{P(y=1)}{1-P(y=1)} = Odds = \exp(\beta_0 + \beta_1 x_1 \ + \beta_2 x_2 + .. + \beta_p x_p)$$

We compare what happens when we increase one of the feature values by 1.

We look at the ratio of the two predictions:

$$\frac{Odds_{x_j+1}}{Odds_{x_j}} = \frac{\exp(\beta_0 + \beta_1 x_1 + .. + \beta_j \ (x_j + 1) + .. + \beta_p x_p)}{\exp(\beta_0 + \beta_1 x_1 + .. + \beta_j x_j + .. + \beta_p x_p)}$$
$$= \exp\big(\beta_j (x_j + 1\big) - \beta_j x_j) = \exp(\beta_j)$$

- If we increase the value of feature $x_j$ by one unit, the estimated odds change by a factor of $\exp(\beta_j)$

# Example - Logistic regression

Let's consider a hypothetical example where we want to predict the likelihood of a student passing an exam based on the number of hours they studied and whether they attended a preparatory course.

$$P(y = 1) = \frac{1}{1 + \exp(-(\beta_0 + \beta_1 Hours\ Studied\ + \beta_2 Preparatory\ Course))}$$

$\beta_0$ = -2, $\beta_1$ = 0.8, $\beta_2$ = 1.2

- For every additional hour studied, the odds of passing the exam increase by approximately 2.22 (≈ e^0.8) times.
- Students who attended a preparatory course have odds 3.32 (≈ e^1.2) times higher of passing the exam compared to those who did not attend the preparatory course, holding the hours studied constant.

# Advantages of Linear/Logistic Regression

- Simple Interpretation
  - Via coefficients

- Provide variable importance
  - Via the magnitude and sign of the coefficients

# Limitations of Linear/Logistic Regression

- Low accuracy compared to more complex model
  - Interpretability accuracy trade-off

- Limited to Linear Decision Boundaries

# Interpreting Naïve Bayes

$$P(C_k|x) = \frac{1}{Z}\,\mathrm{P}(\mathrm{C_k})\prod_{i=1}^{n} P(x_i|C_k)$$

- **Feature Importance**
  - Given by the conditional probabilities of features given the class labels.
  - For each class, Naive Bayes calculates the probability of each feature occurring given that class. Higher probabilities indicate that the feature is more indicative of that class.

# Advantages and Disadvantages of Naïve Bayes

Advantages

- Simple and easy to implement
- Provide feature importance

Disadvantage

- Assumption of Feature Independence
- Limited expressiveness, low performance

# Instance-based classifiers - KNN

- Prediction based on the K nearest neighbors of the instance

- Explanation by example
  - Set instances, the K nearest neighbours

- Do not offer global interpretability
  - It is inherently local!

# Advantages and Limitations of KNN

Advantages

- Easy to derive the explanation

- Explanation by example is close as how often human reason

- Intuitive for some data types
  - e.g., similar images

Disadvantages

- Difficult to interpret as we increase the number of features
- Other form of explanations, e.g., feature importance, could be preferred

# Stages of Explainability – Explainable modelling

- **Targeting interpretability by design**
  - Design high-performing models imposing interpretability constraints to enable their interpretability
  - e.g., Explainability via regularization
    - Apply regularization to improve model explainability

$$\min_{f \in F} \sum_{i} Loss(f, x_i, y_i) + \text{InterpretabilityPenalty}(f),$$

$$\text{subject to Interpretability constraint}(f)$$

Cynthia Rudin et al. “Interpretable machine learning: Fundamental principles and 10 grand challenges”, 2021

# Targeting interpretability by design

- Trees

$$\min_{f \in \text{ set of trees}} \frac{1}{n} \sum_i \text{Loss}(f, z_i) + C \cdot \textbf{Number of leaves } (f),$$

- Linear models

$$\min_{f \in \mathcal{F}} \quad \frac{1}{n} \sum_i \text{Loss}(f, z_i) + C \cdot \text{Number of nonzero terms } (f), \quad \text{subject to}$$

$$f \text{ is a linear model, } f(\mathbf{x}) = \sum_{j=1}^{p} \lambda_j x_j,$$

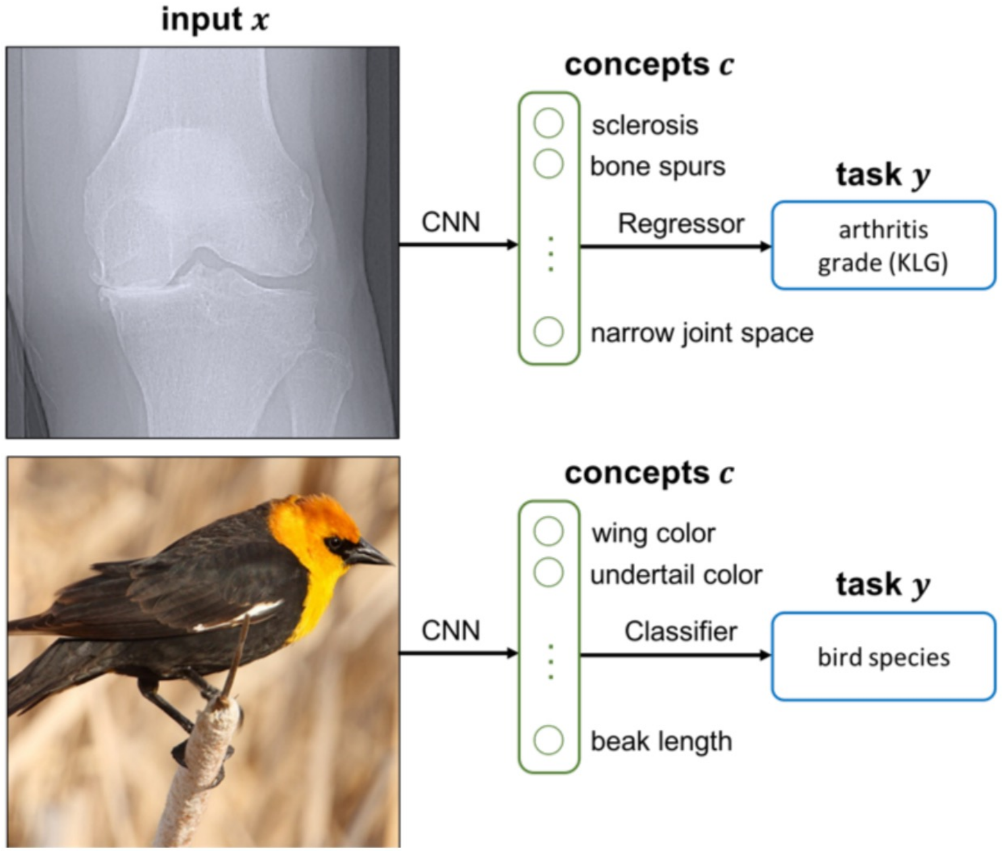
Problem: these models could still underperform compared to more complex models

Cynthia Rudin et al. “Interpretable machine learning: Fundamental principles and 10 grand challenges”, 2021

Wu, Mike, et al. "Beyond sparsity: Tree regularization of deep models for interpretability." AAAI 2018.

# Targeting interpretability by design - Concept-based models

- E.g., Concept Bottleneck Models

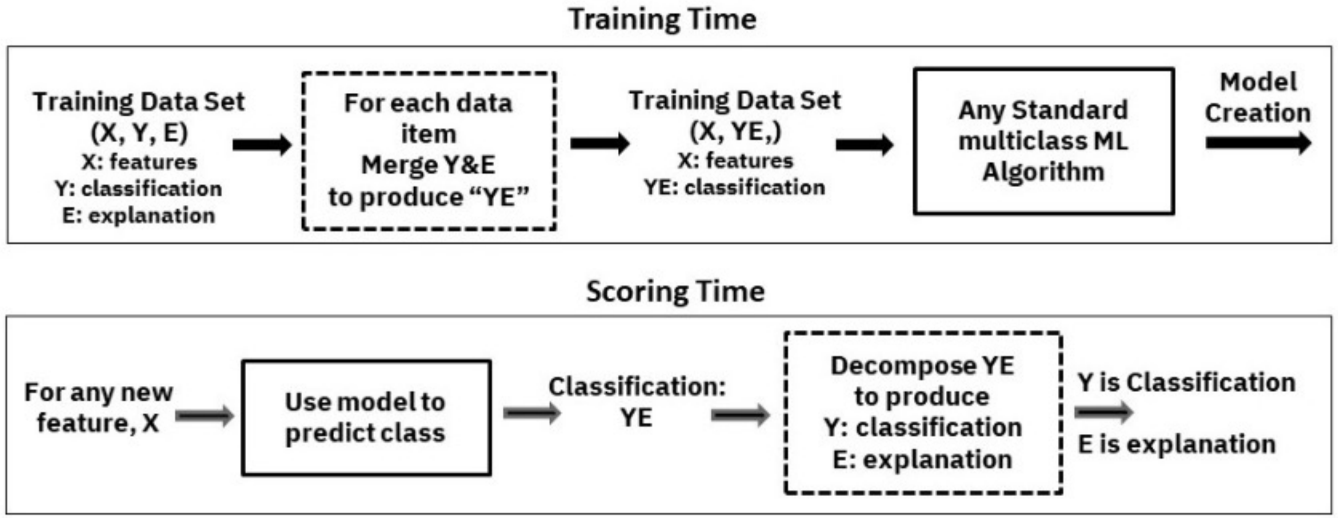


Koh, Pang Wei, et al. "Concept bottleneck models." International conference on machine learning. PMLR, 2020.

# Stages of Explainability – Explainable modelling

- **Explanations-in-the-loop**

  **Train** AI systems **to** jointly **provide** a prediction and its **explanation**



Training Time

Training Data Set
(X, Y, E)
X: features
Y: classification
E: explanation

For each data item
Merge Y&E
to produce "YE"

Training Data Set
(X, YE,)
X: features
YE: classification

Any Standard multiclass ML Algorithm

Model Creation

Scoring Time

For any new feature, X

Use model to predict class

Classification: YE

Decompose YE to produce
Y: classification
E: explanation

Y is Classification

E is explanation

Hind et al. TED: Teaching AI to Explain its Decisions. AIES 2019

# TED - Teaching Explanations for Decisions

Train a model to jointly produce both a decision as well as an explanation

**Analogy – Teaching & Learning process**

- Training: As a supervisor show the new employee several example situations and teach them the correct action: approve or reject a loan application, and explain the reason for the action, such as "insufficient salary".
- Deployment: The new employee will be able to make independent decisions on new loan applications and will give explanation based on the explanations they learned from their supervisor

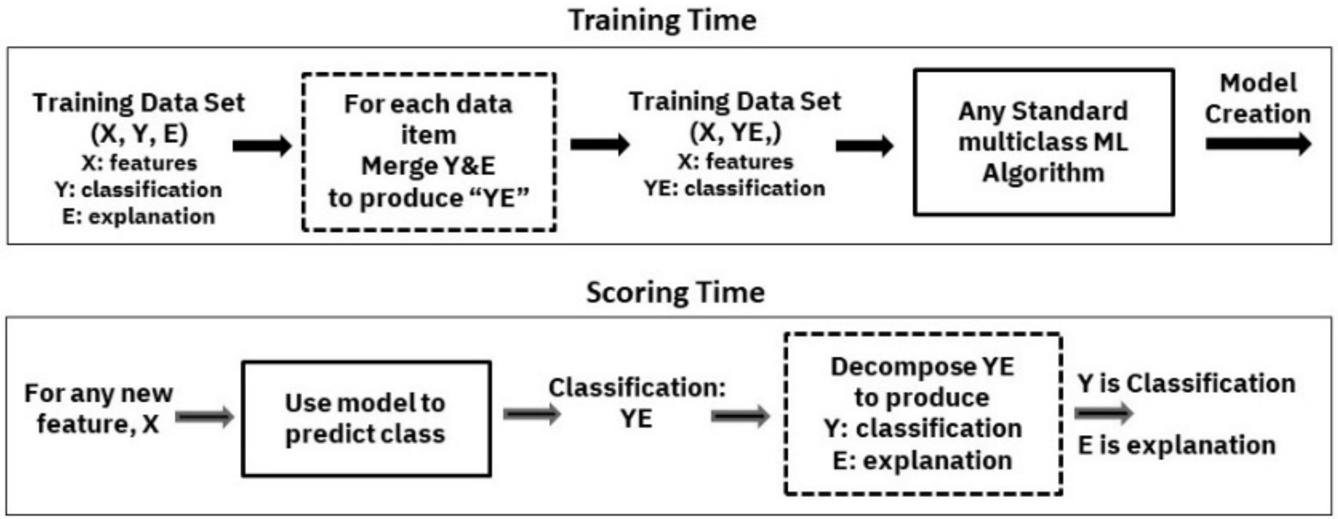
**TED**

- Training: Teach the model to make correct predictions but also to learn their explanations, by providing them
- Test/Deployment: For a new sample, the model generates the prediction and its explanation

Hind et al. TED: Teaching AI to Explain its Decisions. AIES 2019

# TED - Teaching Explanations for Decisions

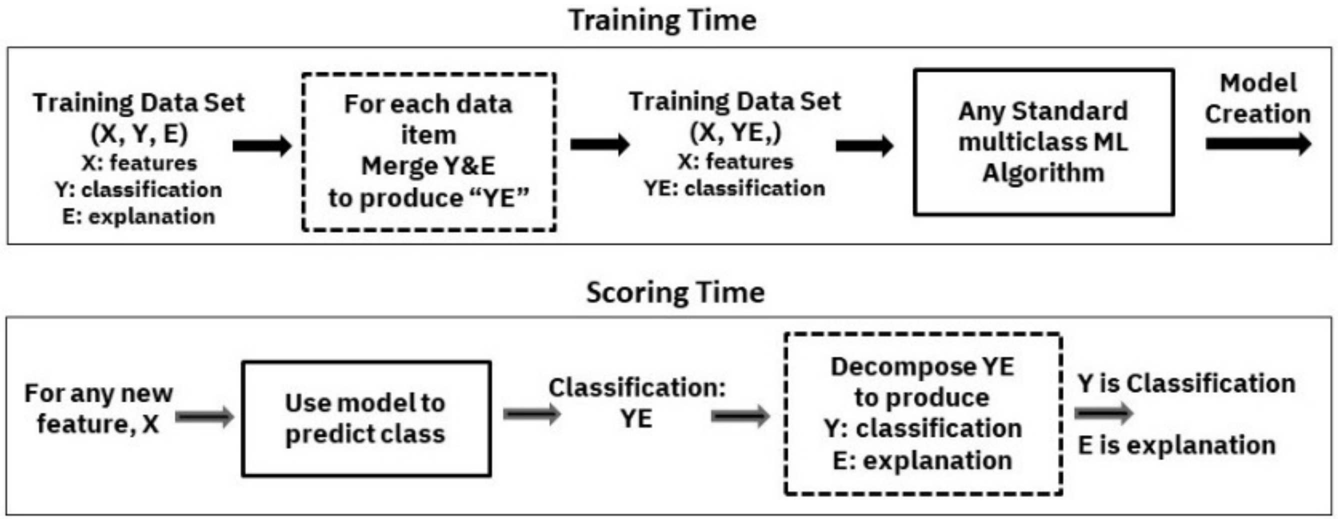
- Training data
  - X, Y, E (Explanation)
  - E is a **rationales:** human annotations that can explain labels, ground truth explanation
- Training
  - Learn Y+E from X
  - Generic classification model f



Hind et al. TED: Teaching AI to Explain its Decisions. AIES 2019

# TED - Teaching Explanations for Decisions

- Test/Deployment
  - Predict Y+E from new instances
  - Decompose Y, E



Training Time

Training Data Set (X, Y, E)
X: features
Y: classification
E: explanation

For each data item Merge Y&E to produce "YE"

Training Data Set (X, YE,)
X: features
YE: classification

Any Standard multiclass ML Algorithm

Model Creation

Scoring Time

For any new feature, X

Use model to predict class

Classification: YE

Decompose YE to produce
Y: classification
E: explanation

Y is Classification

E is explanation

Hind et al. TED: Teaching AI to Explain its Decisions. AIES 2019

# Advantages of Explanation-in-the-loop

- Explainability directly in the training process

- Teach the model what important for us as human
  - Alignment to human reasoning and values

- Explanation can be tailored for the target audience

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# Limitations of Explanation-in-the-loop

- Require a dataset annotated with explanations
  - The paper tests the approach with synthetic rationales..
    - Rationales as rules and predict which one matches the input, encoded as an integer

- Explanations may not necessarily reflect of how model predictions were made but what humans expects

- Faithfulness to the model vs Plausibility
  - Faithfulness: whether the explanation matches the model inner working
  - Plausibility: whether the explanation matches what humans expect

Hind et al. TED: Teaching AI to Explain its Decisions. AIES 2019

# Teach Me to Explain – Datasets annotated with explanations

- Goal
  - to train better models via additional training supervision
  - to train interpretable models that explain their own predictions
  - to evaluate *plausibility* of model-generated explanations by measuring their agreement with human explanations

- Multiple examples, especially for text data
  - Highlight – part of the input --> What a **wonderful** day! Sentiment: positive
  - Free text --> ‘The answer is correct because the person said it with a joyful voice’
  - Structured --> e.g., constrained text/form ’Is it joyful? Yes/no’ Yes, ‘Is it loud?’ Yes

Wiegreffe, Sarah, and Ana Marasovic. "Teach Me to Explain: A Review of Datasets for Explainable Natural Language Processing.” Neurips Benchmark and Datasets 2021

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