

Workshop in XGBOOST and Multitemporal DETER Data for Deforestation Forecasting

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Objectives



Method



Environment Setup



Data loading



Train and Evaluation



Interpretability



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Project scope: Produce biweekly deforestation risk maps incorporating data on forest degradation and deforestation from the DETER System and a wide range of socio-political and economic factors.

Main Objectives of the Workshop

- Understand and Set Up the Technical Environment
- Explore the Code Pipeline for Spatiotemporal Modeling
- Model train and evaluation
- Inference and Generate Predictive Maps
- Enable Operationalization and Reproducibility



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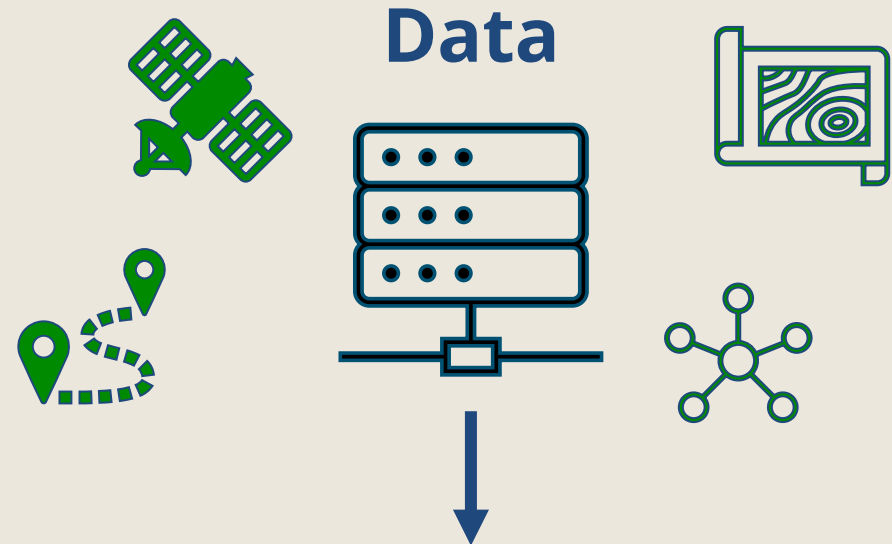
Data loading



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Interpretability

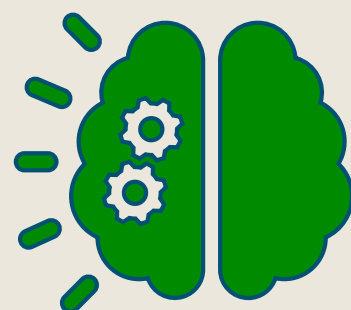


Data

Model



Decision Forest



Neural Network

Risk Map





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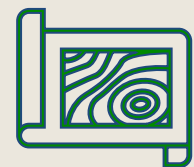
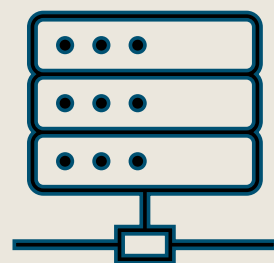
Train and Evaluation



Interpretability



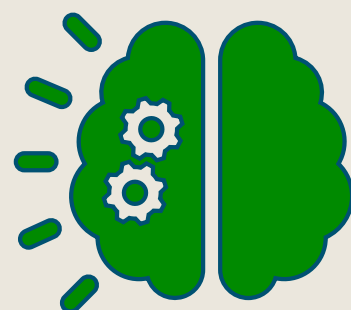
Data



Model



Decision Forest



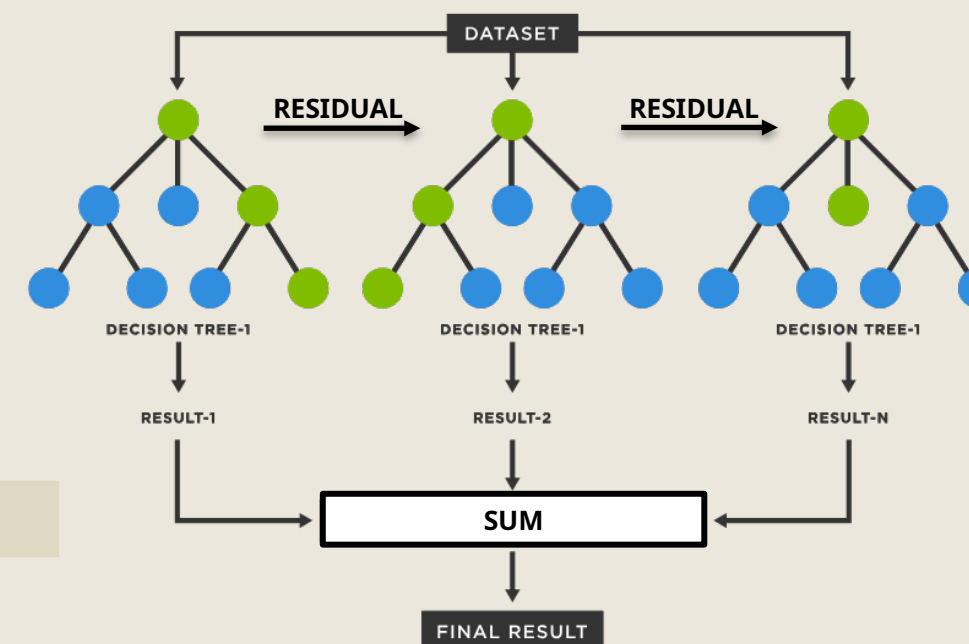
Neural Network



Risk Map



XGBoost



high performance on sparse data

requires less data for accurate results

higher interpretability

requires more modest computational resources

XGBoost builds an ensemble of decision trees rooted in the gradient-boosting paradigm



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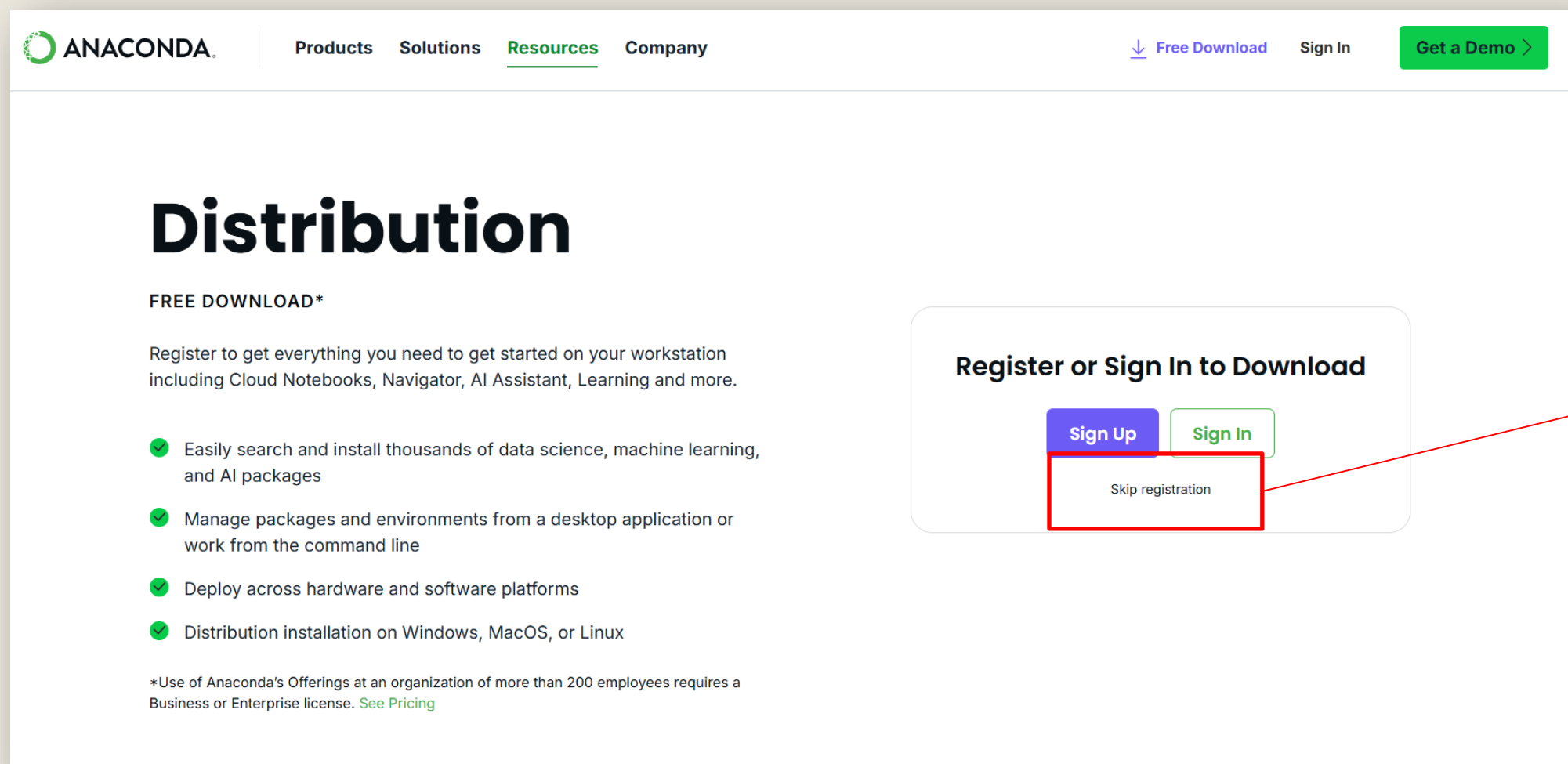


Interpretability

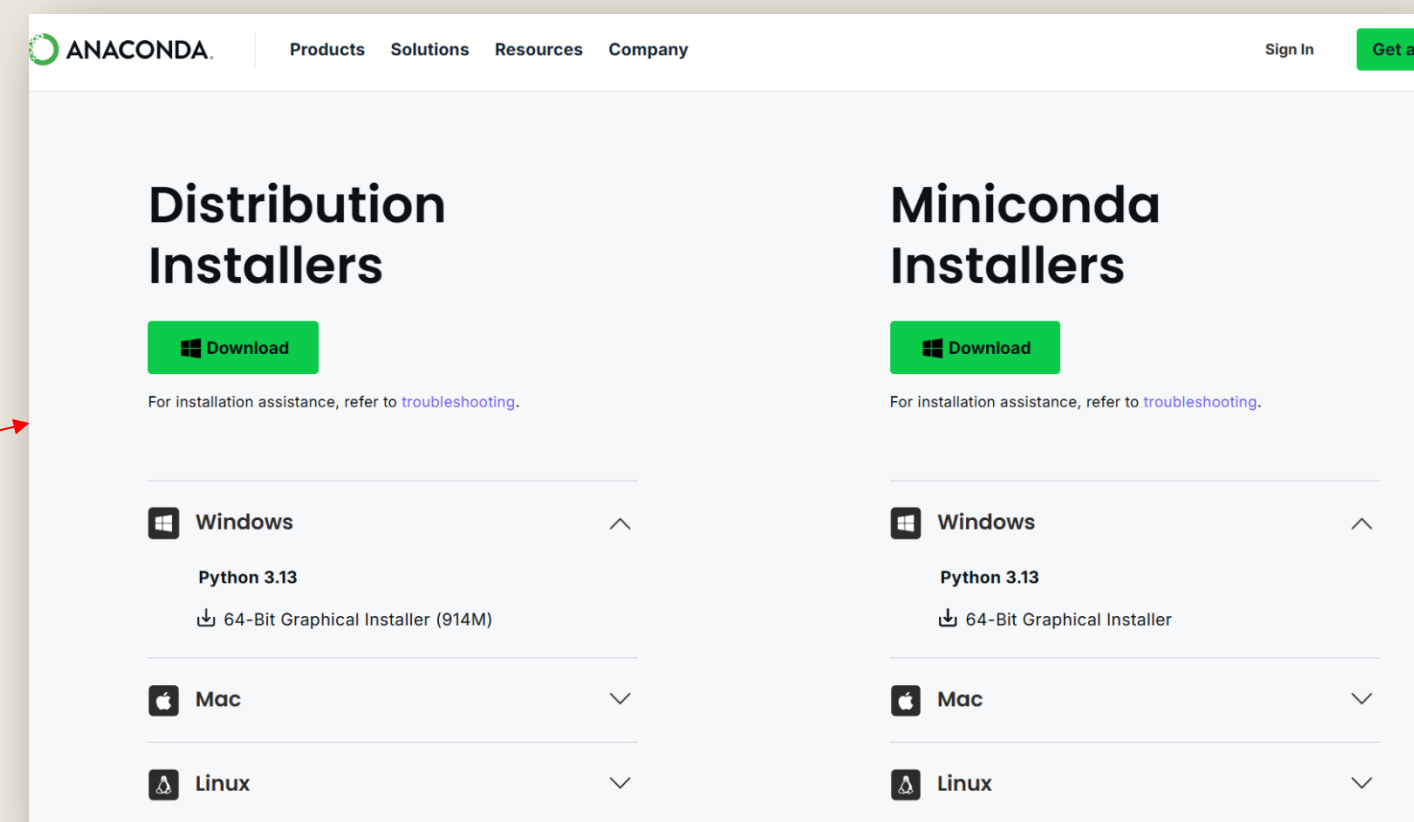
Step-by-Step: Conda + Jupyter + Packages

1. Install Required Tools (if not already installed)

- Download Conda from: <https://www.anaconda.com/download>



The screenshot shows the Anaconda website's 'Distribution' page. The header includes the Anaconda logo and navigation links: Products, Solutions, Resources (highlighted), and Company. On the right, there are links for 'Free Download', 'Sign In', and a 'Get a Demo' button. The main heading is 'Distribution' with a subheading 'FREE DOWNLOAD*'. Below this, a paragraph states: 'Register to get everything you need to get started on your workstation including Cloud Notebooks, Navigator, AI Assistant, Learning and more.' A list of four bullet points follows, each with a green checkmark: 'Easily search and install thousands of data science, machine learning, and AI packages', 'Manage packages and environments from a desktop application or work from the command line', 'Deploy across hardware and software platforms', and 'Distribution installation on Windows, MacOS, or Linux'. At the bottom left, a small note mentions that use at organizations with more than 200 employees requires a Business or Enterprise license. On the right side of the page, a box titled 'Register or Sign In to Download' contains three buttons: 'Sign Up' (purple), 'Sign In' (green), and 'Skip registration' (white with a red border). A red arrow points from the 'Skip registration' button to the 'Distribution Installers' section of the next screenshot.



The screenshot shows the 'Distribution Installers' page on the Anaconda website. The header is similar to the previous page, with the Anaconda logo and navigation links. On the right, there are links for 'Sign In' and a 'Get a Demo' button. The main heading is 'Distribution Installers'. Below the heading is a green 'Download' button with a Windows icon. A link for 'troubleshooting' is provided. The page is divided into two columns: 'Distribution Installers' and 'Miniconda Installers'. Each column has a 'Download' button and a 'troubleshooting' link. Below these, there are sections for 'Windows', 'Mac', and 'Linux'. Each section lists the operating system, the Python version (Python 3.13), and the installer type (64-Bit Graphical Installer) with a download icon and file size (914M).



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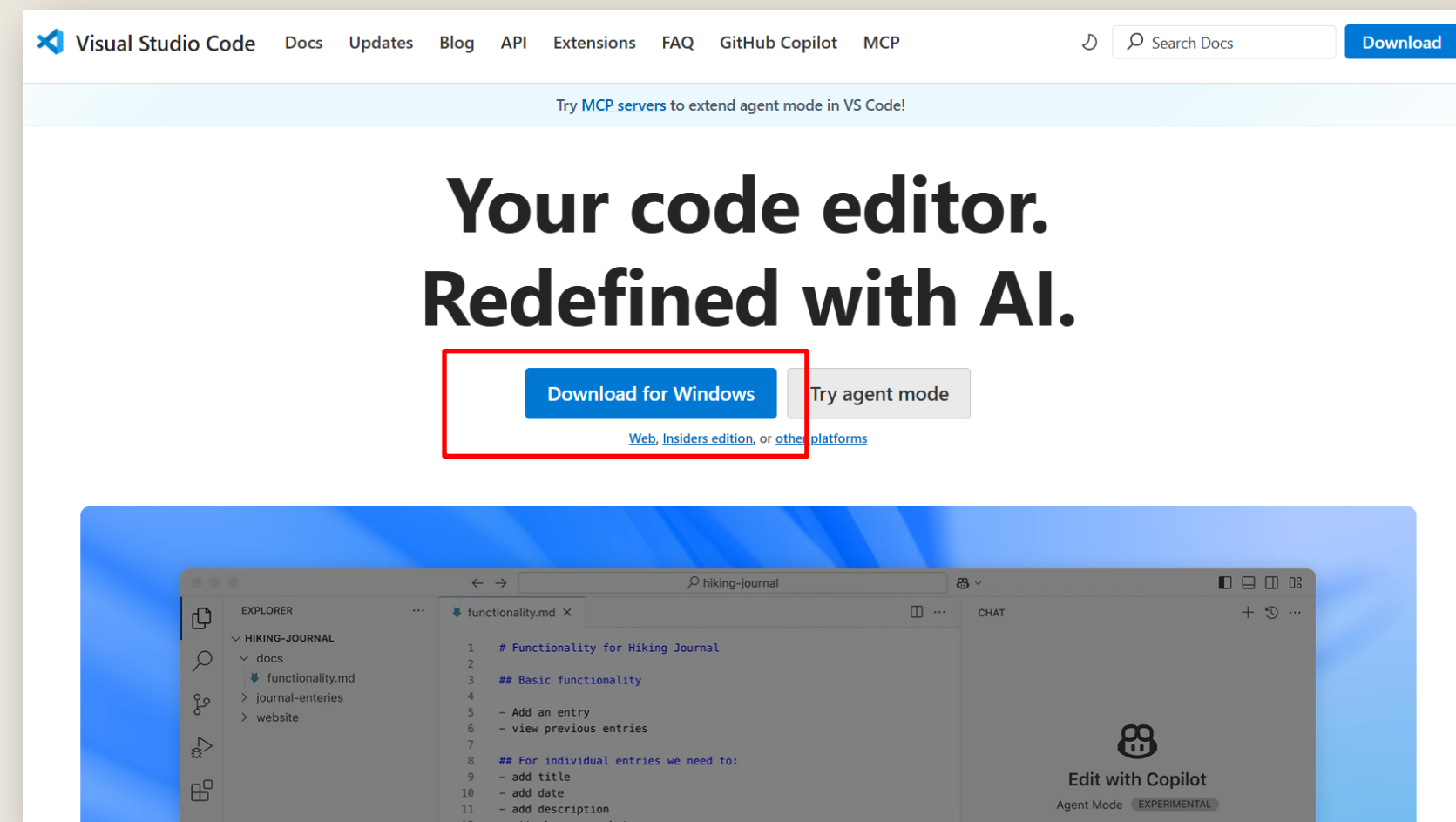
Interpretability

Step-by-Step: Conda + Jupyter + Packages

1. Install Required Tools (if not already installed)

- Download Conda from: <https://www.anaconda.com/download>
- Download VS Code from: <https://code.visualstudio.com/>

Run the installer and follow the default installation steps





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Interpretability

Step-by-Step: Conda + Jupyter + Packages

1. Install Required Tools (if not already installed)

- Download Conda from: <https://www.anaconda.com/download>

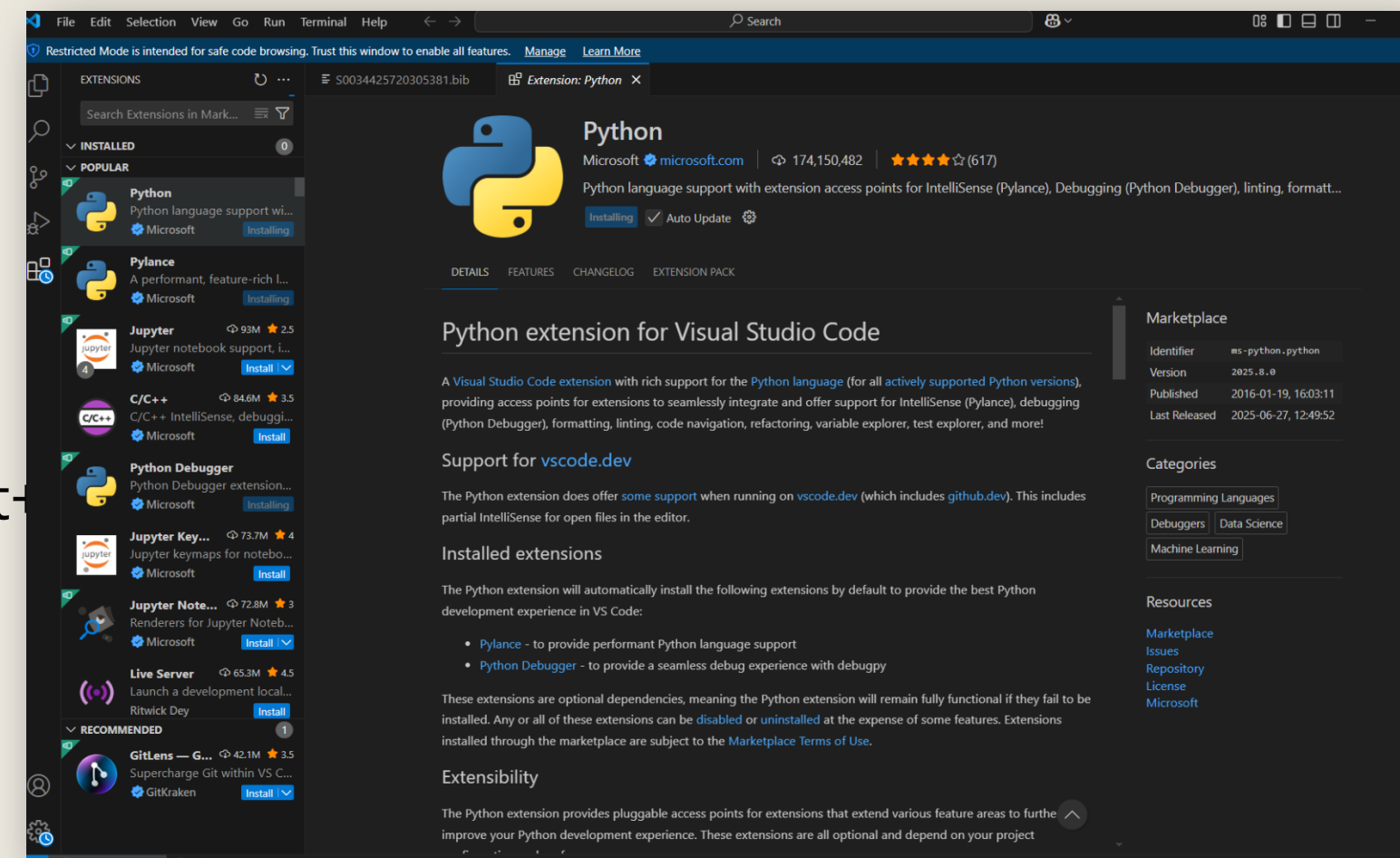
- Download VS Code from: <https://code.visualstudio.com/>

- Install Python Extension

1. Click the Extensions icon in the Activity Bar (or press Ctrl+Shift-X)
2. Search for "Python" (by Microsoft)
3. Click "Install"

- Install Jupyter Notebook Extension

1. Click the Extensions icon in the Activity Bar (or press Ctrl+Shift+X)
2. Search for "Jupyter" (by Microsoft)
3. Click "Install"





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Interpretability

Step-by-Step: Conda + Jupyter + Packages

 1. Install Required Tools (if not already installed)

 2. Create and Configure a Conda Environment

- Open **Anaconda Prompt** or a terminal and type



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Interpretability

Step-by-Step: Conda + Jupyter + Packages

1. Install Required Tools (if not already installed)

2. Create and Configure a Conda Environment

- Open **Anaconda Prompt** or a terminal and type

```
# 1. Create a new Conda environment with Python 3.10
conda create -n xgboost_env python=3.10 -y

# 2. Activate the environment
conda activate xgboost_env

# 3. Install the required packages from conda-forge
conda install -c conda-forge \
    numpy=1.26.4 \
    gdal=3.6.2 \
    xgboost \
    scikit-learn \
    scikit-image \
    matplotlib \
    pandas \
    rasterio \
    requests \
    shap \
    wheel \
    setuptools \
    jupyterlab \
    pystac \
    seaborn -y
```




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Step-by-Step: Conda + Jupyter + Packages

 1. Install Required Tools (if not already installed)

 2. Create and Configure a Conda Environment

 3. Open the Project in VS Code

- Launch VS Code
- Open your project folder: **File → Open Folder → Select the project directory**



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Interpretability

Step-by-Step: Conda + Jupyter + Packages

 1. Install Required Tools (if not already installed)

 2. Create and Configure a Conda Environment

 3. Open the Project in VS Code

 4. Set VS Code Python Interpreter

- Press Ctrl+Shift+P
- Type: Python: Select Interpreter
- Select: xgboost_env (conda)



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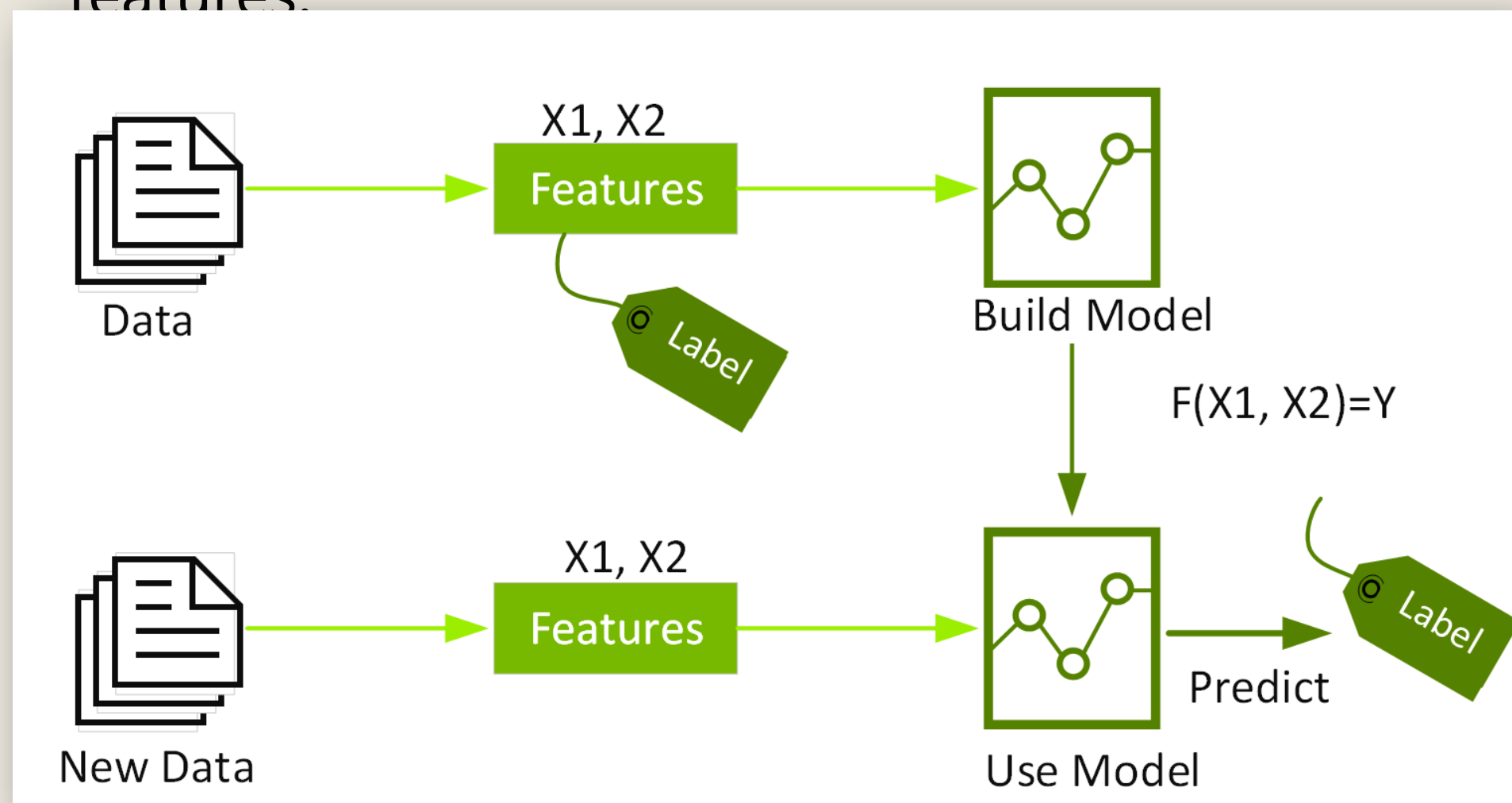
Train and Evaluation



Interpretability

What is XGBoost?

- Supervised machine learning uses algorithms to train a model to find **patterns** in a dataset with **labels** and **features** and then uses the trained model to **predict** the labels on a **new** dataset's features.



$$\text{obj}(\theta) = L(\theta) + \Omega(\theta)$$

$$L(\theta) = \sum_i (y_i - \hat{y}_i)^2$$



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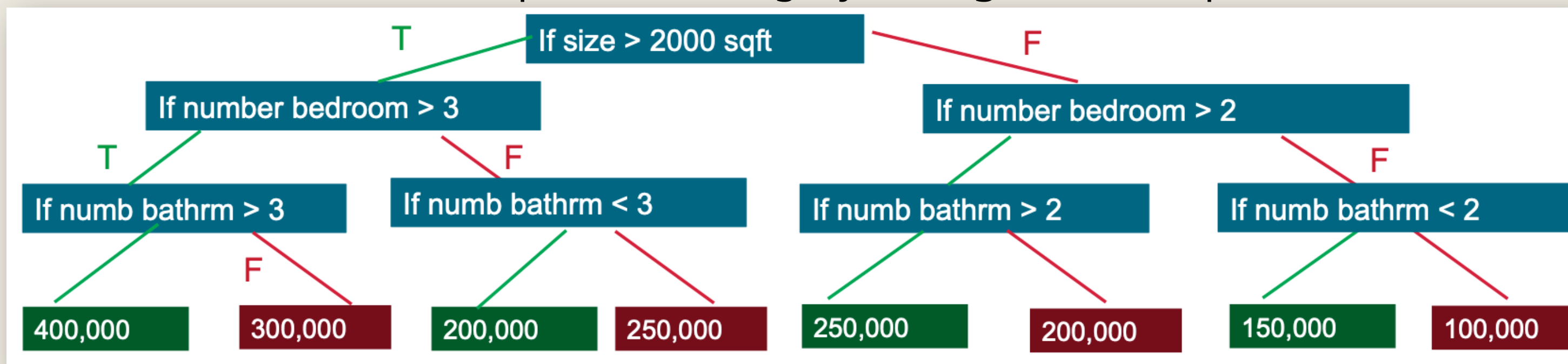
Train and Evaluation



Interpretability

What is XGBoost?

- Predicts the label by evaluating a tree of **if-then-else true/false** feature questions
- Estimates the **minimum** number of questions needed to assess the probability of making a correct decision
- Can be used for **classification** to predict a category, or **regression** to predict a continuous numeric value





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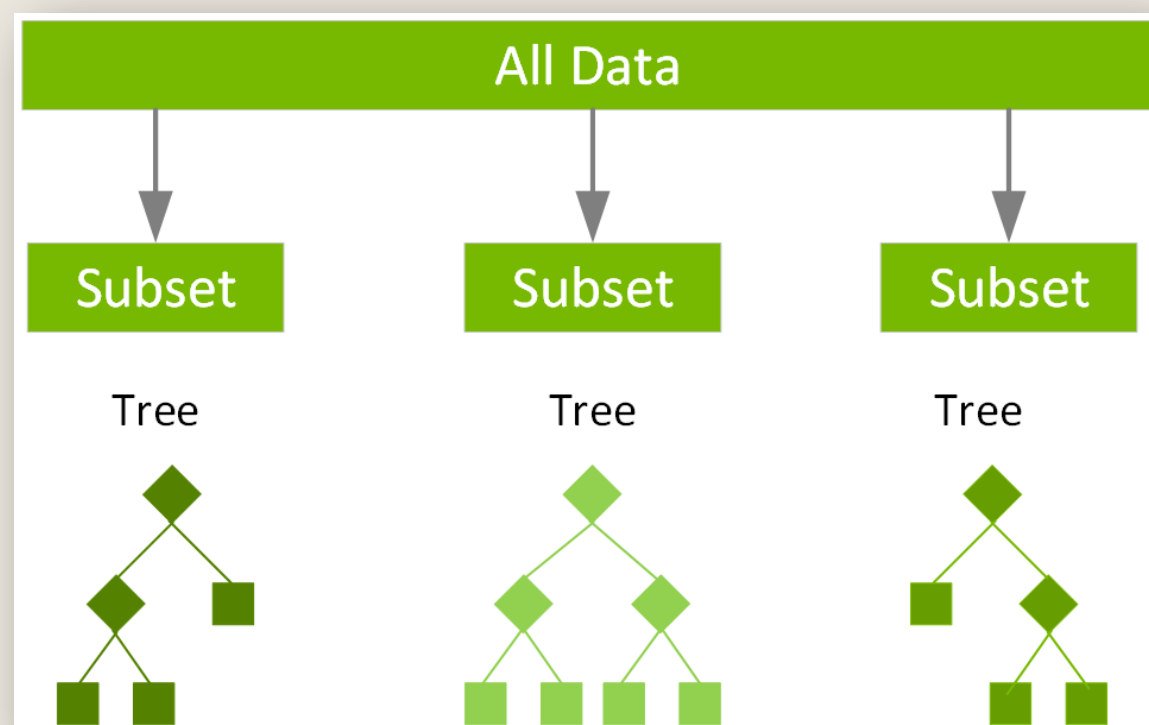
Train and Evaluation



Interpretability

What is XGBoost?

- **Ensembles** -> combine the decisions from multiple models to improve the overall performance.





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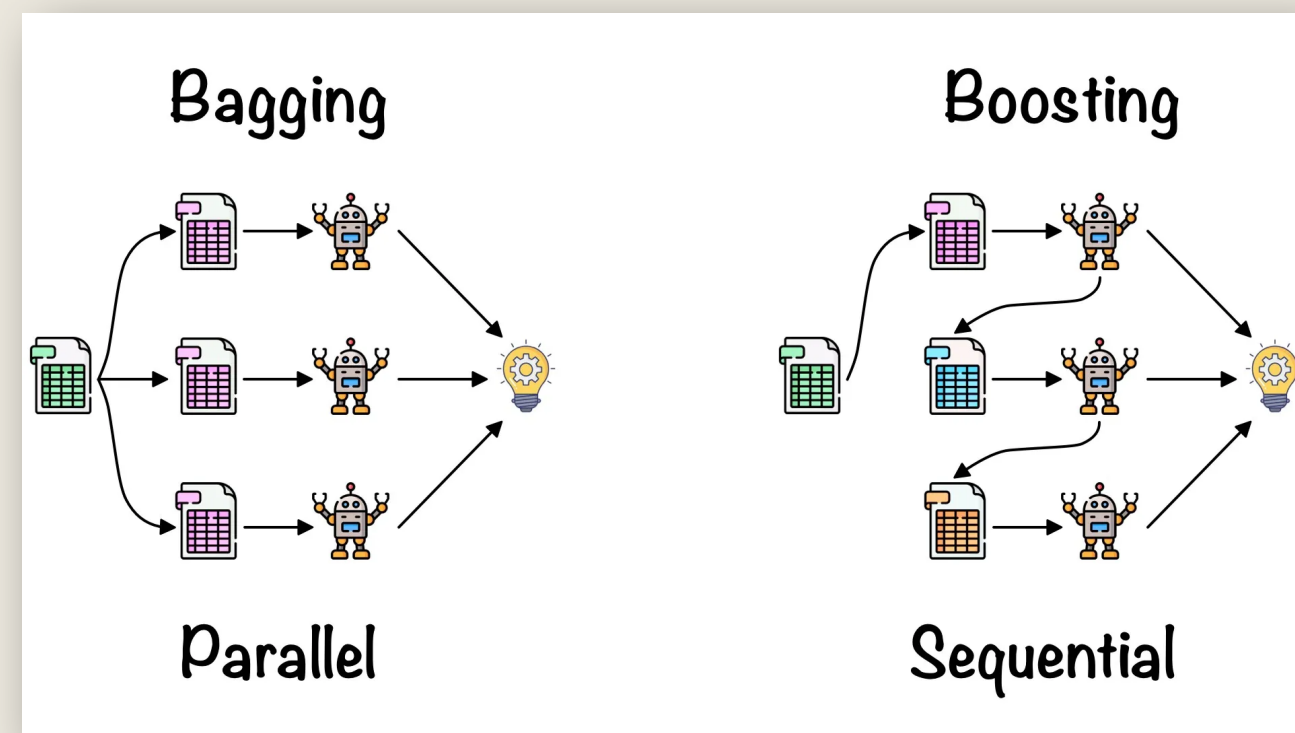
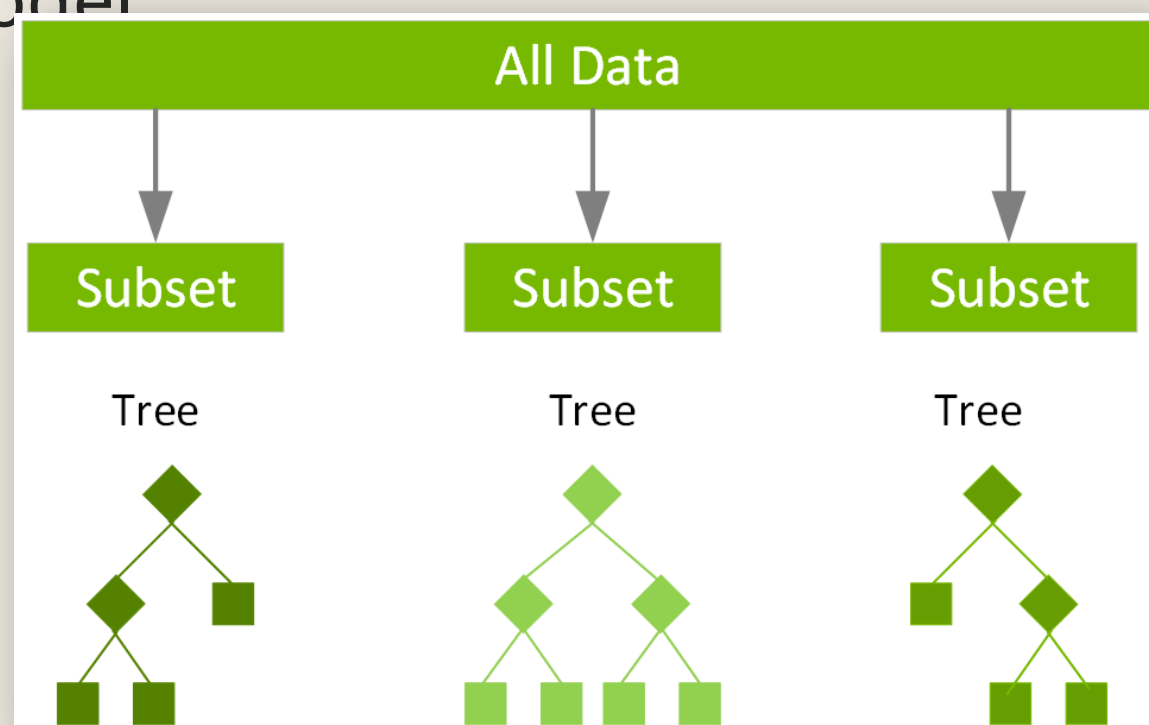
Train and Evaluation



Interpretability

What is XGBoost?

- **Ensembles** -> combine the decisions from multiple models to improve the overall performance.
- **BAGGING** -> subsetting the data and aggregating the results (e.g, Random Forest)
- **BOOSTING** -> sequential, each subsequent model attempts to correct the errors of the previous model





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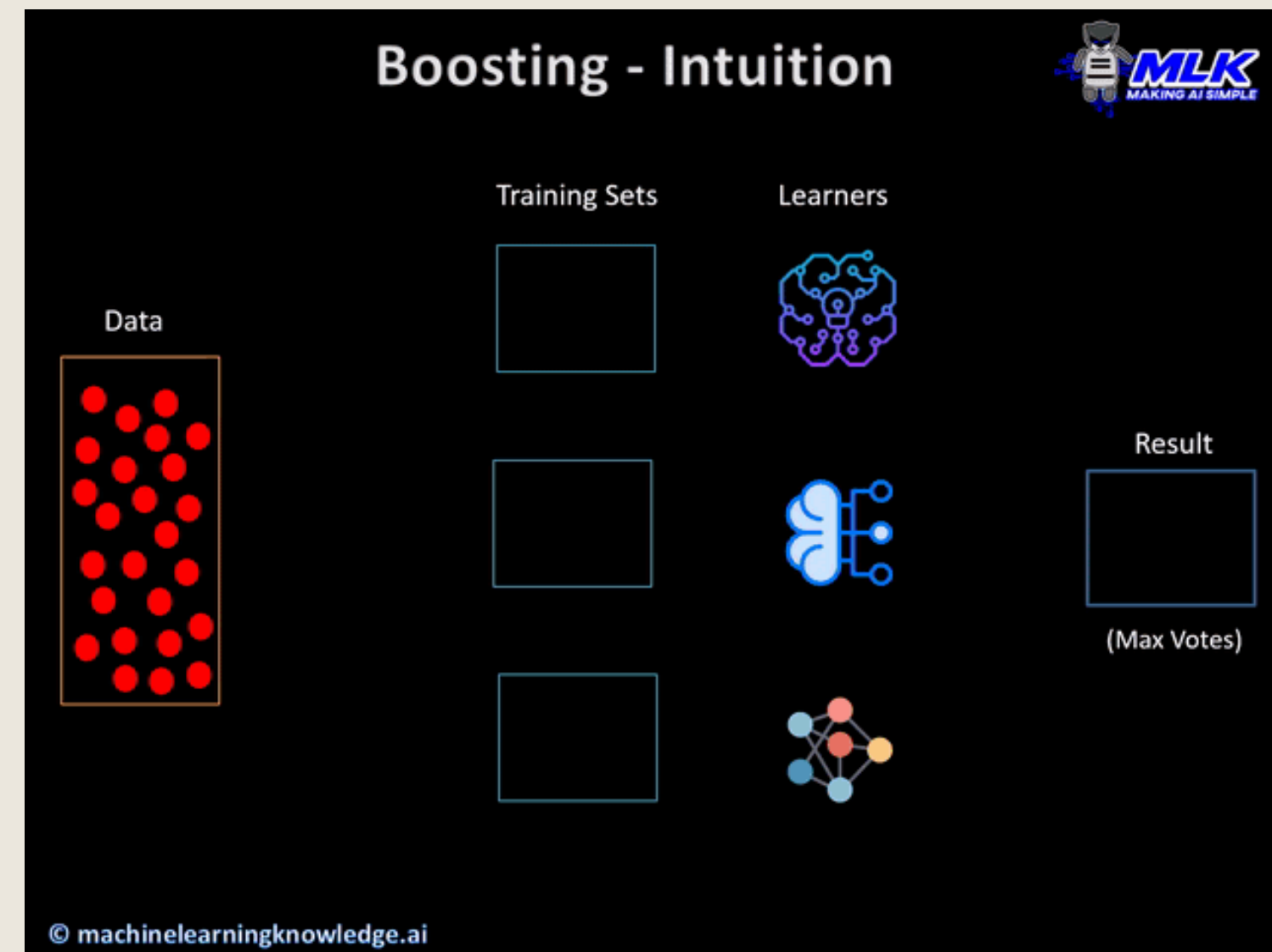


Interpretability

What is XGBoost?

GRADIENT BOOSTING

- Improving a single weak model by combining it with a number of other weak models -> Collectively strong model
- Each decision tree within the committee is specifically trained to address the residual errors propagated by the preceding trees





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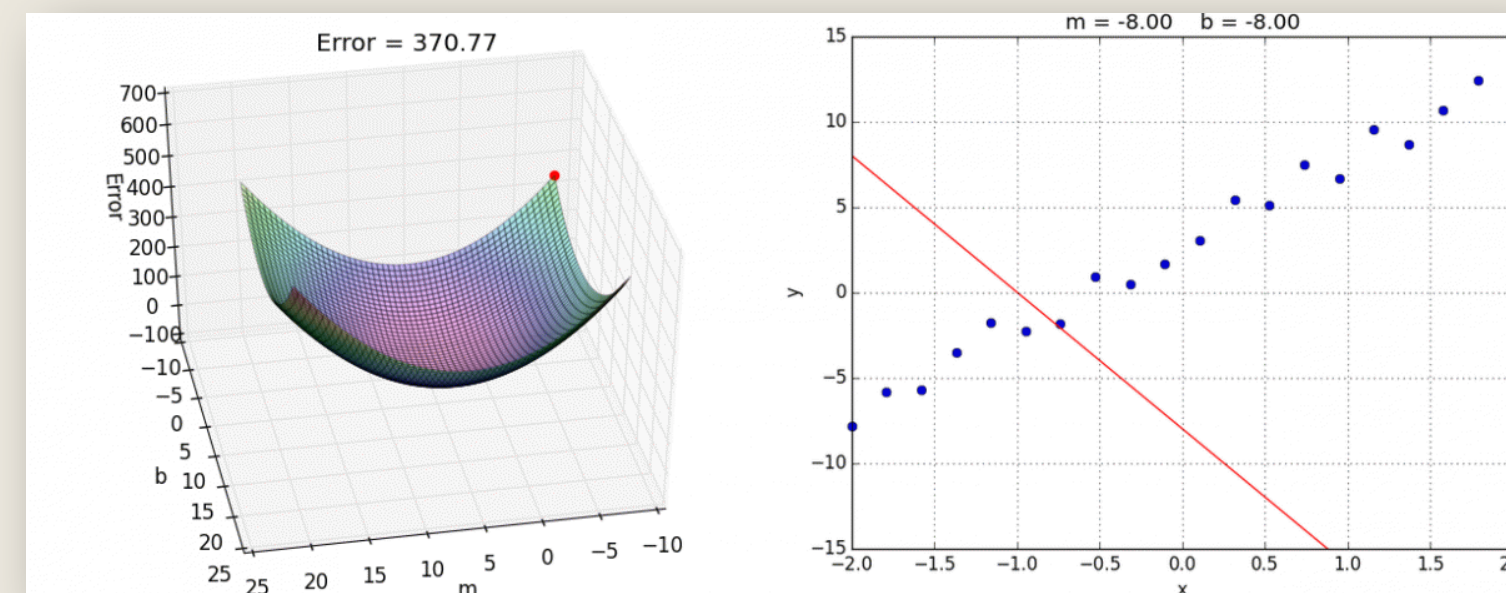


Interpretability

What is XGBoost?

GRADIENT BOOSTING

- Improving a single weak model by combining it with a number of other weak models -> Collectively strong model
- Each decision tree within the committee is specifically trained to address the residual errors propagated by the preceding trees
- The gradient of the loss function guides this correction
- The training involves assigning weights to each tree based on their contribution





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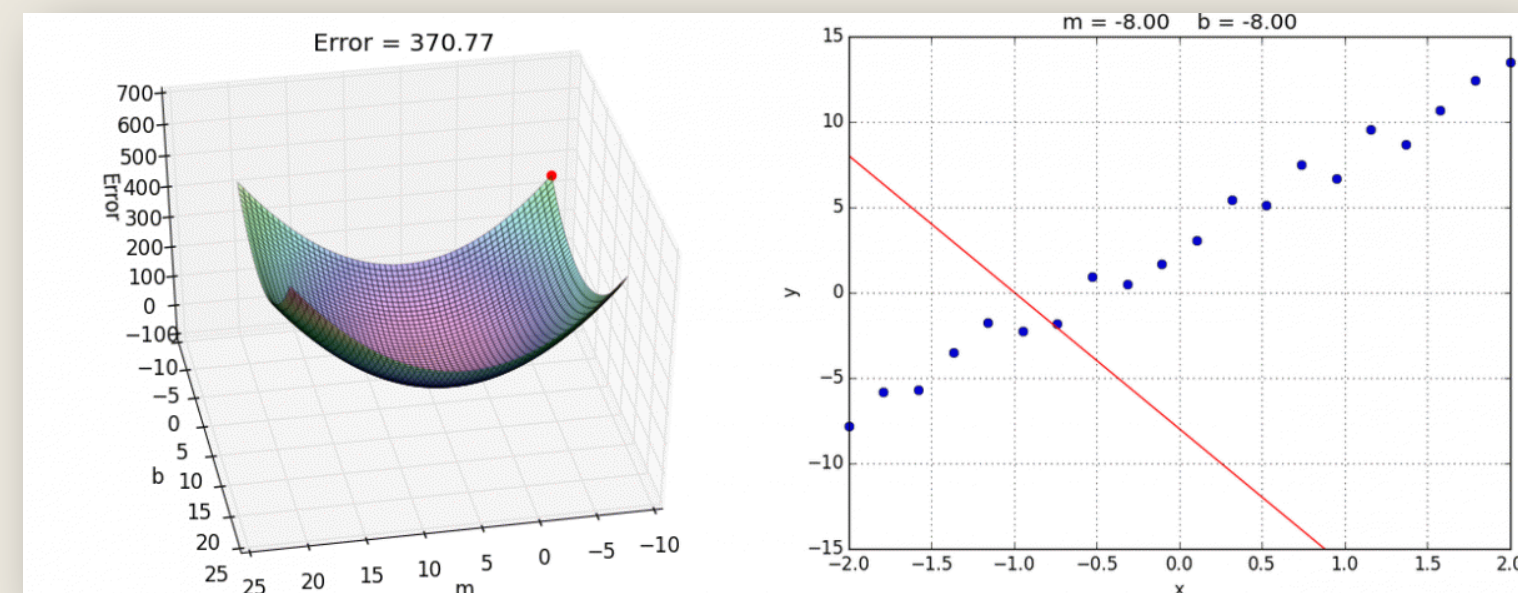
Interpretability

What is XGBoost?

GRADIENT BOOSTING

- In order to minimize the loss function we take the derivative of the loss function and add the negative of this value to the weight scaled by some learning rate to achieve a more accurate model this process is repeated until convergence.

$$\theta^{(m+1)} = \theta^{(m)} - \text{learningRate} * \frac{\partial L}{\partial \theta^{(m)}}$$





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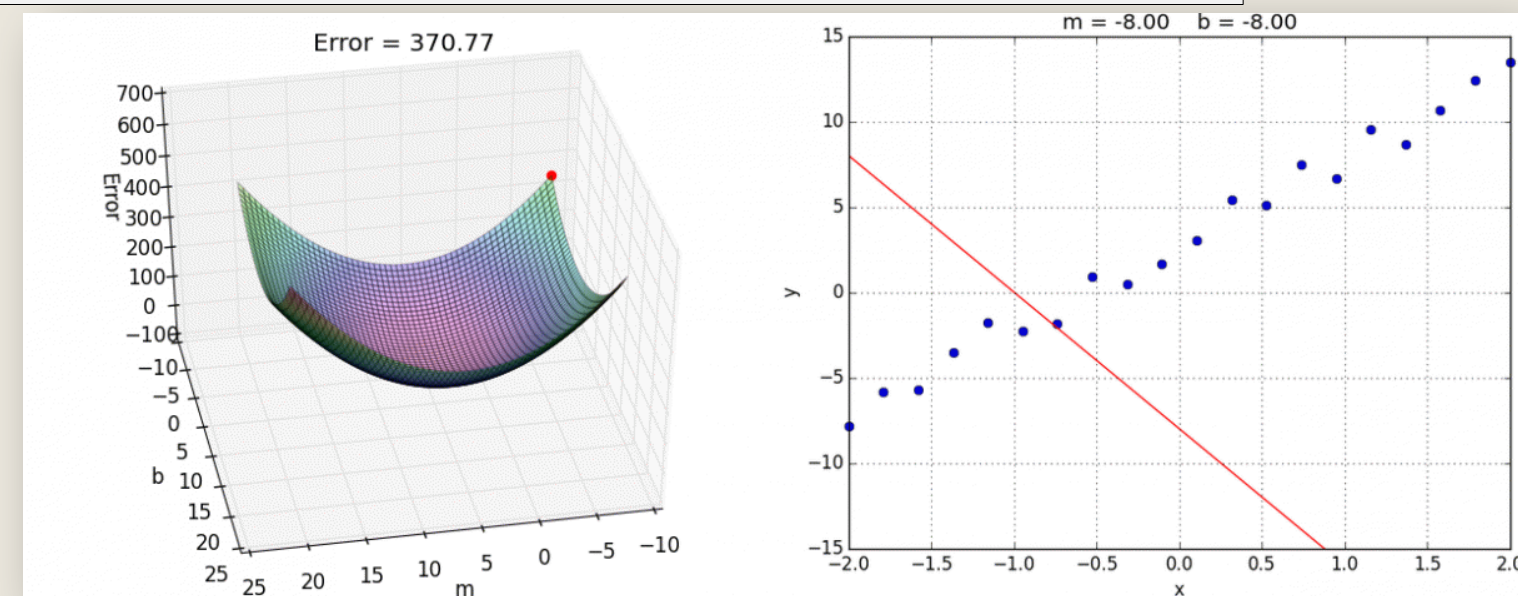


Interpretability

XGBoost is a scalable and highly accurate implementation of gradient boosting

GRADIENT BOOSTING

- In order to minimize the loss function we take the derivative of the loss function and add the negative of this value to the weight scaled by some learning rate to achieve a more accurate model this process is repeated until convergence.



$$\theta^{(m+1)} = \theta^{(m)} - \text{learningRate} * \frac{\partial L}{\partial \theta^{(m)}}$$



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Interpretability

Why XGBoost?

- **Regularization:** penalize complex models through both L1 and L2 regularization. Regularization helps in preventing overfitting.
- **Handling sparse data:** sparsity-aware split finding algorithm to handle different types of sparsity patterns in the data.
- **Weighted quantile sketch:** Most existing tree-based algorithms can find the split points when the data points are of equal weights (using a quantile sketch algorithm). However, they are not equipped to handle weighted data. XGBoost has a distributed weighted quantile sketch algorithm to effectively handle weighted data
- **Block structure for parallel learning:** make use of multiple cores on the CPU.



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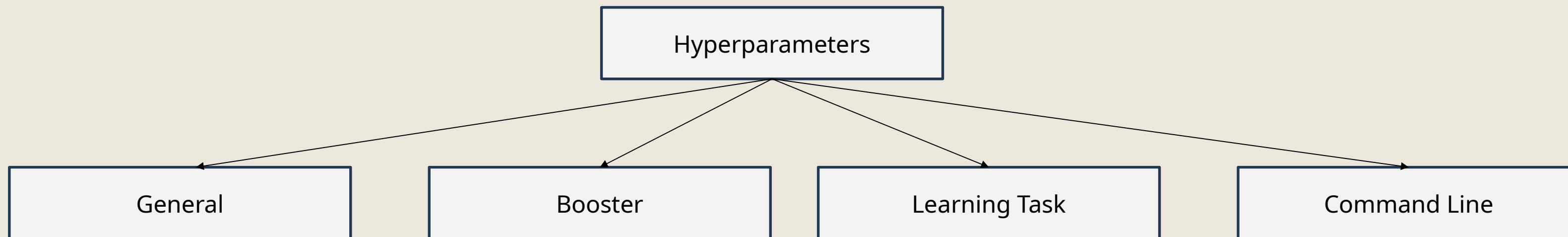


Train and Evaluation



Interpretability

Hyperparameters in XGBoost





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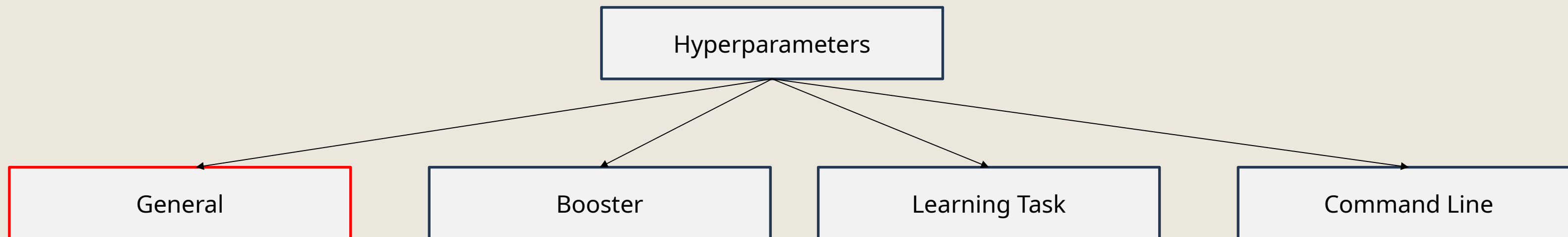


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Hyperparameters in XGBoost

General

- `nthread` [default to maximum number of threads available if not set]
 - Number of parallel threads used to run XGBoost. When choosing it, please keep thread contention and hyperthreading in mind.

- `booster` [default= `gbtree`]
 - Which booster to use. Can be `gbtree`, `gblinear` or `dart`; `gbtree` and `dart` use tree based models while `gblinear` uses linear functions.

- `device` [default= `cpu`]

Added in version 2.0.0.

- Device for XGBoost to run. User can set it to one of the following values:
 - `cpu`: Use CPU.
 - `cuda`: Use a GPU (CUDA device).
 - `cuda:<ordinal>`: `<ordinal>` is an integer that specifies the ordinal of the GPU (which GPU do you want to use if you have more than one devices).
 - `gpu`: Default GPU device selection from the list of available and supported devices. Only `cuda` devices are supported currently.
 - `gpu:<ordinal>`: Default GPU device selection from the list of available and supported devices. Only `cuda` devices are supported currently.

For more information about GPU acceleration, see [XGBoost GPU Support](#). In distributed environments, ordinal selection is handled by distributed frameworks instead of XGBoost. As a result, using `cuda:<ordinal>` will result in an error. Use `cuda` instead.

- `verbosity` [default=1]
 - Verbosity of printing messages. Valid values are 0 (silent), 1 (warning), 2 (info), 3 (debug). Sometimes XGBoost tries to change configurations based on heuristics, which is displayed as warning message. If there's unexpected behaviour, please try to increase value of verbosity.



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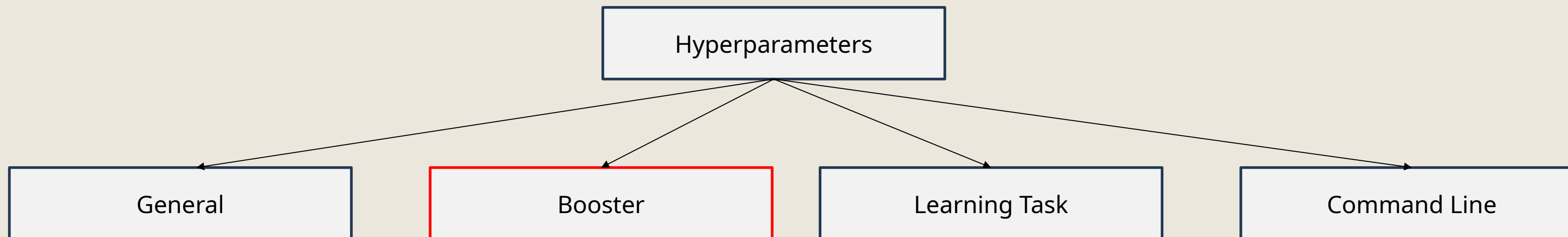


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Booster

- `min_child_weight` [default=1]
 - Minimum sum of instance weight (hessian) needed in a child. If the tree partition step results in a leaf node with the sum of instance weight less than `min_child_weight`, then the building process will give up further partitioning. In linear regression task, this simply corresponds to minimum number of instances needed to be in each node. The larger `min_child_weight` is, the more conservative the algorithm will be.
 - range: $[0, \infty]$
- `subsample` [default=1]
 - Subsample ratio of the training instances. Setting it to 0.5 means that XGBoost would randomly sample half of the training data prior to growing trees. and this will prevent overfitting. Subsampling will occur once in every boosting iteration.
 - range: $(0, 1]$

- `eta` [default=0.3, alias: `learning_rate`]
 - Step size shrinkage used in update to prevent overfitting. After each boosting step, we can directly get the weights of new features, and `eta` shrinks the feature weights to make the boosting process more conservative.
 - range: $[0, 1]$
- `gamma` [default=0, alias: `min_split_loss`]
 - Minimum loss reduction required to make a further partition on a leaf node of the tree. The larger `gamma` is, the more conservative the algorithm will be. Note that a tree where no splits were made might still contain a single terminal node with a non-zero score.
 - range: $[0, \infty]$
- `max_depth` [default=6, type=int32]
 - Maximum depth of a tree. Increasing this value will make the model more complex and more likely to overfit. 0 indicates no limit on depth. Beware that XGBoost aggressively consumes memory when training a deep tree. `exact` tree method requires non-zero value.
 - range: $[0, \infty]$



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Booster

- `lambda` [default=1, alias: `reg_lambda`]
 - L2 regularization term on weights. Increasing this value will make model more conservative.
 - range: $[0, \infty]$
- `alpha` [default=0, alias: `reg_alpha`]
 - L1 regularization term on weights. Increasing this value will make model more conservative.
 - range: $[0, \infty]$

- `colsample_bytree`, `colsample_bylevel`, `colsample_bynode` [default=1]
 - This is a family of parameters for subsampling of columns.
 - All `colsample_by*` parameters have a range of $(0, 1]$, the default value of 1, and specify the fraction of columns to be subsampled.
 - `colsample_bytree` is the subsample ratio of columns when constructing each tree. Subsampling occurs once for every tree constructed.
 - `colsample_bylevel` is the subsample ratio of columns for each level. Subsampling occurs once for every new depth level reached in a tree. Columns are subsampled from the set of columns chosen for the current tree.
 - `colsample_bynode` is the subsample ratio of columns for each node (split). Subsampling occurs once every time a new split is evaluated. Columns are subsampled from the set of columns chosen for the current level. This is not supported by the exact tree method.
 - `colsample_by*` parameters work cumulatively. For instance, the combination `{'colsample_bytree':0.5, 'colsample_bylevel':0.5, 'colsample_bynode':0.5}` with 64 features will leave 8 features to choose from at each split.

Using the Python or the R package, one can set the `feature_weights` for DMatrix to define the probability of each feature being selected when using column sampling. There's a similar parameter for `fit` method in sklearn interface.



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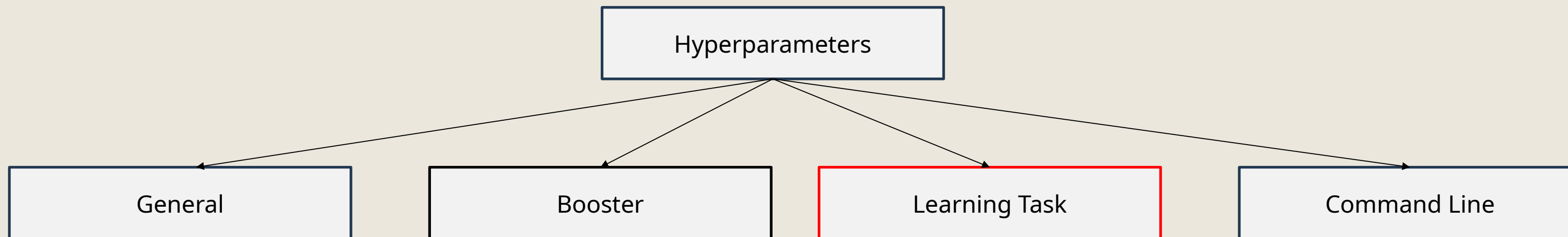


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Learning Task

- `objective` [default=reg:squarederror]
 - `reg:squarederror`: regression with squared loss.
 - `reg:squaredlogerror`: regression with squared log loss $\frac{1}{2} [\log(pred + 1) - \log(label + 1)]^2$. All input labels are required to be greater than -1. Also, see metric `rmsle` for possible issue with this objective.
 - `reg:logistic`: logistic regression, output probability
 - `reg:pseudohubererror`: regression with Pseudo Huber loss, a twice differentiable alternative to absolute loss.
 - `reg:absoluteerror`: Regression with L1 error. When tree model is used, leaf value is refreshed after tree construction. If used in distributed training, the leaf value is calculated as the mean value from all workers, which is not guaranteed to be optimal.
Added in version 1.7.0.
 - `reg:quantileerror`: Quantile loss, also known as `pinball loss`. See later sections for its parameter and [Quantile Regression](#) for a worked example.
Added in version 2.0.0.
 - `binary:logistic`: logistic regression for binary classification, output probability
 - `binary:logitraw`: logistic regression for binary classification, output score before logistic transformation
 - `binary:hinge`: hinge loss for binary classification. This makes predictions of 0 or 1, rather than producing probabilities.
 - `count:poisson`: Poisson regression for count data, output mean of Poisson distribution.
 - `max_delta_step` is set to 0.7 by default in Poisson regression (used to safeguard



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Learning Task

- `survival:cox`: Cox regression for right censored survival time data (negative values are considered right censored). Note that predictions are returned on the hazard ratio scale (i.e., as $HR = \exp(\text{marginal_prediction})$ in the proportional hazard function $h(t) = h_0(t) * HR$).
- `survival:aft`: Accelerated failure time model for censored survival time data. See [Survival Analysis with Accelerated Failure Time](#) for details.
- `multi:softmax`: set XGBoost to do multiclass classification using the softmax objective, you also need to set `num_class`(number of classes)
- `multi:softprob`: same as softmax, but output a vector of `ndata * nclass`, which can be further reshaped to `ndata * nclass` matrix. The result contains predicted probability of each data point belonging to each class.
- `rank:ndcg`: Use LambdaMART to perform pair-wise ranking where [Normalized Discounted Cumulative Gain \(NDCG\)](#) is maximized. This objective supports position debiasing for click data.
- `rank:map`: Use LambdaMART to perform pair-wise ranking where [Mean Average Precision \(MAP\)](#) is maximized
- `rank:pairwise`: Use LambdaRank to perform pair-wise ranking using the *ranknet* objective.
- `reg:gamma`: gamma regression with log-link. Output is a mean of gamma distribution. It might be useful, e.g., for modeling insurance claims severity, or for any outcome that might be [gamma-distributed](#).
- `reg:tweedie`: Tweedie regression with log-link. It might be useful, e.g., for modeling total loss in insurance, or for any outcome that might be [Tweedie-distributed](#).



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Learning Task

- `eval_metric` [default according to objective]

- Evaluation metrics for validation data, a default metric will be assigned according to objective (rmse for regression, and logloss for classification, *mean average precision* for `rank:map`, etc.)
- User can add multiple evaluation metrics. Python users: remember to pass the metrics in as list of parameters pairs instead of map, so that latter `eval_metric` won't override previous ones
- The choices are listed below:
 - `rmse`: [root mean square error](#)
 - `rmsle`: root mean square log error: $\sqrt{\frac{1}{N} [\log(pred + 1) - \log(label + 1)]^2}$. Default metric of `reg:squaredlogerror` objective. This metric reduces errors generated by outliers in dataset. But because `log` function is employed, `rmsle` might output `nan` when prediction value is less than -1. See `reg:squaredlogerror` for other requirements.
 - `mae`: [mean absolute error](#)
 - `mape`: [mean absolute percentage error](#)
 - `mphe`: [mean Pseudo Huber error](#). Default metric of `reg:pseudohubererror` objective.
 - `logloss`: [negative log-likelihood](#)
 - `error`: Binary classification error rate. It is calculated as $\frac{\#(wrong\ cases)}{\#(all\ cases)}$. For the predictions, the evaluation will regard the instances with prediction value larger than 0.5 as positive instances, and the others as negative instances.
 - `error@t`: a different than 0.5 binary classification threshold value could be specified by providing a numerical value through 't'.
 - `merror`: Multiclass classification error rate. It is calculated as $\frac{\#(wrong\ cases)}{\#(all\ cases)}$.
 - `mlogloss`: [Multiclass logloss](#).
 - `auc`: [Receiver Operating Characteristic Area under the Curve](#). Available for classification and learning-to-rank tasks.



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Learning Task

- `seed` [default=0]
 - Random number seed. In the R package, if not specified, instead of defaulting to seed 'zero', will take a random seed through R's own RNG engine.

- `aucpr` : Area under the PR curve. Available for classification and learning-to-rank tasks.

After XGBoost 1.6, both of the requirements and restrictions for using `aucpr` in classification problem are similar to `auc`. For ranking task, only binary relevance label $y \in [0, 1]$ is supported. Different from `map` (mean average precision), `aucpr` calculates the *interpolated* area under precision recall curve using continuous interpolation.

- `pre` : Precision at k . Supports only learning to rank task.
- `ndcg` : Normalized Discounted Cumulative Gain
- `map` : Mean Average Precision

The *average precision* is defined as:

$$AP@l = \frac{1}{\min(l, N)} \sum_{k=1}^l P@k \cdot I_{(k)}$$

where $I_{(k)}$ is an indicator function that equals to 1 when the document at k is relevant and 0 otherwise. The $P@k$ is the precision at k , and N is the total number of relevant documents. Lastly, the *mean average precision* is defined as the weighted average across all queries.

- `ndcg@n`, `map@n`, `pre@n` : n can be assigned as an integer to cut off the top positions in the lists for evaluation.
- `ndcg-`, `map-`, `ndcg@n-`, `map@n-` : In XGBoost, the NDCG and MAP evaluate the score of a list without any positive samples as 1. By appending "-" to the evaluation metric name, we can ask XGBoost to evaluate these scores as 0 to be consistent under some conditions.
- `poisson-nloglik` : negative log-likelihood for Poisson regression
- `gamma-nloglik` : negative log-likelihood for gamma regression
- `cox-nloglik` : negative partial log-likelihood for Cox proportional hazards regression
- `gamma-deviance` : residual deviance for gamma regression



Objectives



Method



Environment Setup



Data loading

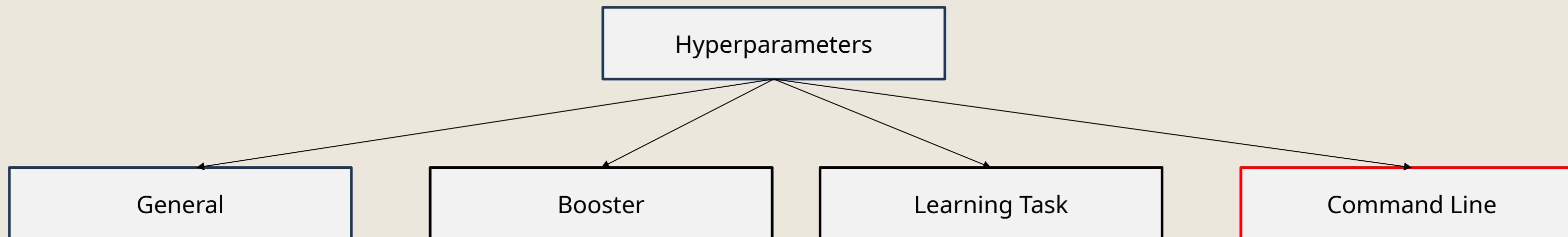


Train and Evaluation



Interpretability

Hyperparameters in XGBoost





Objectives



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Data loading



Train and Evaluation



Interpretability

Hyperparameters in XGBoost

Command Line

- `num_round`
 - The number of rounds for boosting
- `data`
 - The path of training data
- `test:data`
 - The path of test data to do prediction
- `save_period` [default=0]
 - The period to save the model. Setting `save_period=10` means that for every 10 rounds XGBoost will save the model. Setting it to 0 means not saving any model during the training.
- `task` [default= `train`] options: `train`, `pred`, `eval`, `dump`
 - `train`: training using data
 - `pred`: making prediction for test:data
 - `eval`: for evaluating statistics specified by `eval[name]=filename`
 - `dump`: for dump the learned model into text format
- `model_in` [default=NULL]
 - Path to input model, needed for `test`, `eval`, `dump` tasks. If it is specified in training, XGBoost will continue training from the input model.
- `model_out` [default=NULL]
 - Path to output model after training finishes. If not specified, XGBoost will output files with such names as `0003.model` where `0003` is number of boosting rounds.
- `model_dir` [default= `models/`]
 - The output directory of the saved models during training



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Train and Evaluation



Interpretability

Hyperparameters in XGBoost

```
model_reg = xgb.XGBRegressor()
param_grid = {
    'n_estimators': [10, 20, 50, 100, 200, 300, 400, 500],
    'learning_rate': [0.01, 0.05, 0.1, 0.2, 0.3],
    'max_depth': [2, 4, 6, 8, 10],
    'subsample': [0.6, 0.7, 0.8, 0.9, 1.0],
    'min_child_weight': [1, 2, 3, 4, 5],
    'gamma': [0, 0.1, 0.2, 0.3, 0.4],
    'colsample_bytree': [0.6, 0.7, 0.8, 0.9, 1.0],
    'objective': ['reg:gamma', 'reg:squarederror', 'reg:squaredlogerror',
                  'reg:tweedie', 'reg:pseudohubererror']
}

n_iter = 50 # Number of iterations for RandomizedSearchCV
cv_folds = 10 # Cross-validation folds

# Hyperparameter optimization
random_cv = RandomizedSearchCV(
    estimator=model_reg,
    param_distributions=param_grid,
    n_iter=n_iter,
    cv=cv_folds,
    verbose=2,
    random_state=31,
    n_jobs=-1
)
random_cv.fit(train_inputs_reshaped, train_targets_reshaped)
params = random_cv.best_params_
```

```
logging.info("Best Parameters {}".format(params))

# Number of boosting rounds
num_boost_round = 500

# Calculate training time
start_train_time = time.time()

# Train the model
best_model = xgb.train(params, dtrain, num_boost_round, evals=[(dval, 'eval')], early_stopping_rounds=50)

end_train_time = time.time()
train_time = end_train_time - start_train_time
logging.info("Training Time: {:.2f} seconds".format(train_time))
```




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Interpretability

Downloading data from repository



6. Use Jupyter Notebook

- In the conda environment go to the project directory using: `cd "project directory"`
- Type "jupyter lab"
- Open the 01_Data_Acquisition_and>Loading.ipynb notebook

