Tuning Hyperparameters Using Cross Validation Scores

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Overview

Hyperparameter tuning in model validation

Model parameters vs. model hyperparameters

Hyperparameter tuning using Azure ML Studio

Hyperparameters

Model configuration properties that define a model, and remain constant during the training of the model

Hyperparameters

Can be thought of as part of model design

Understanding Hyperparameters

Model Inputs

Model Parameters

Model Hyperparameters

Understanding Hyperparameters

Model Inputs

Input data points, training dataset

Model Parameters

Model Hyperparameters

Understanding Hyperparameters

Model Inputs

Input data points, training dataset

Model Parameters

Structure of decision tree

Model Hyperparameters

Understanding Hyperparameters

Model Inputs

Input data points, training dataset

Model Parameters

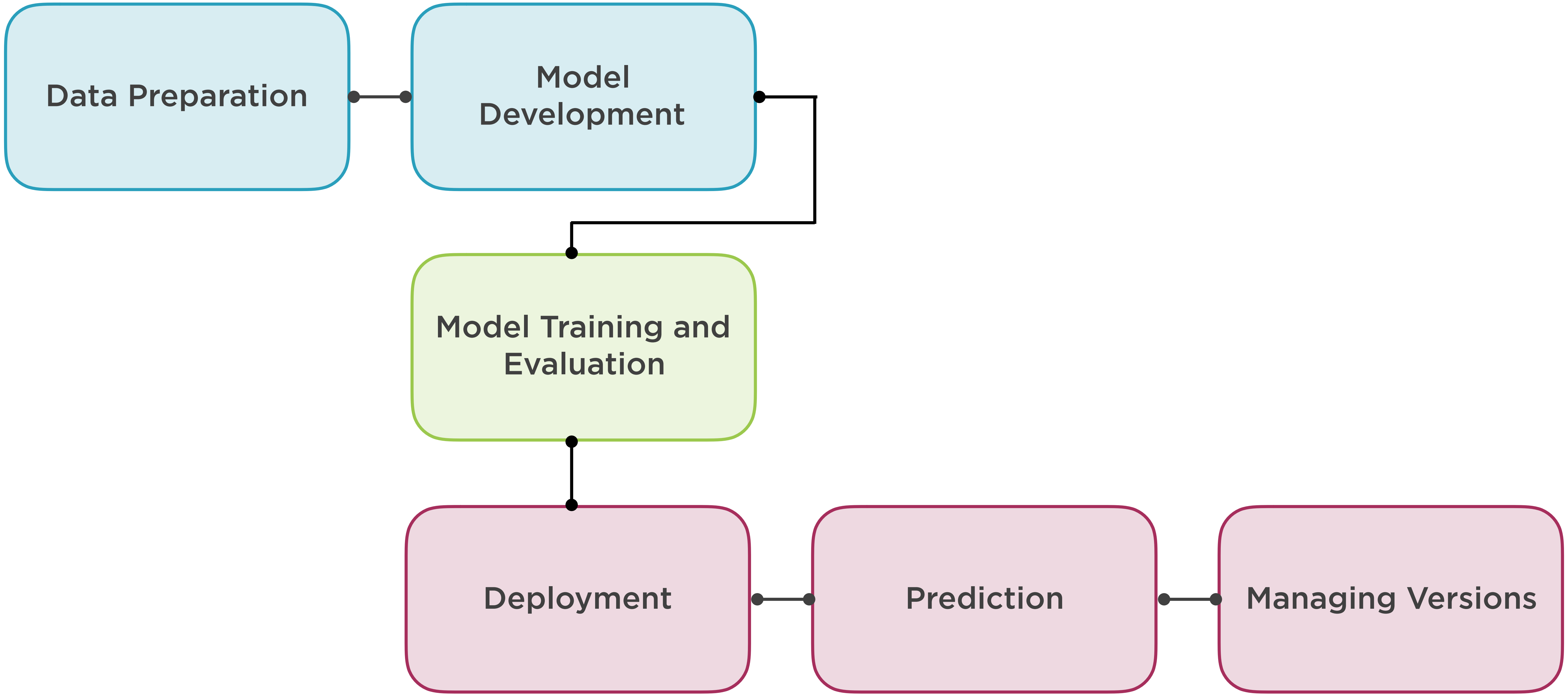
Structure of decision tree

Model Hyperparameters

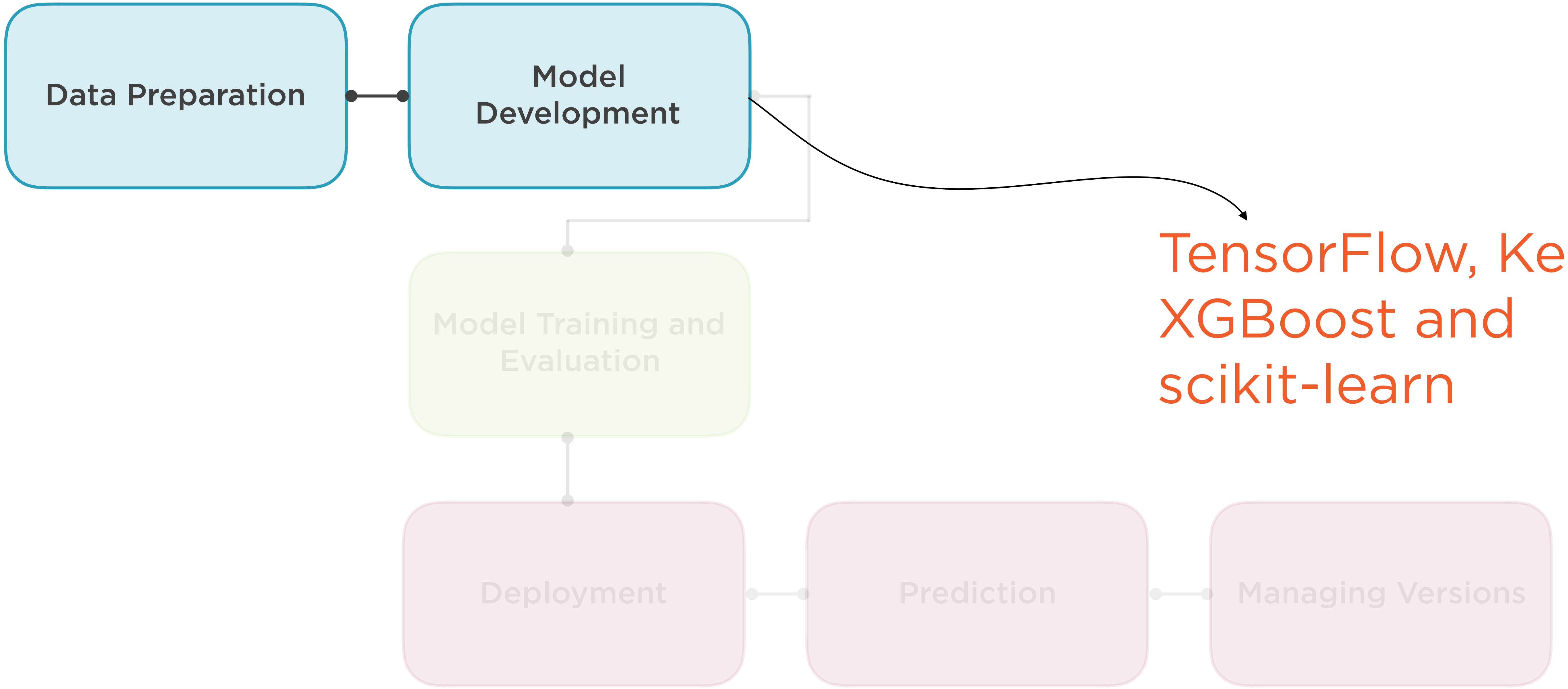
Depth of tree, minimum number of samples per node

Hyperparameter Tuning

Machine Learning Workflow

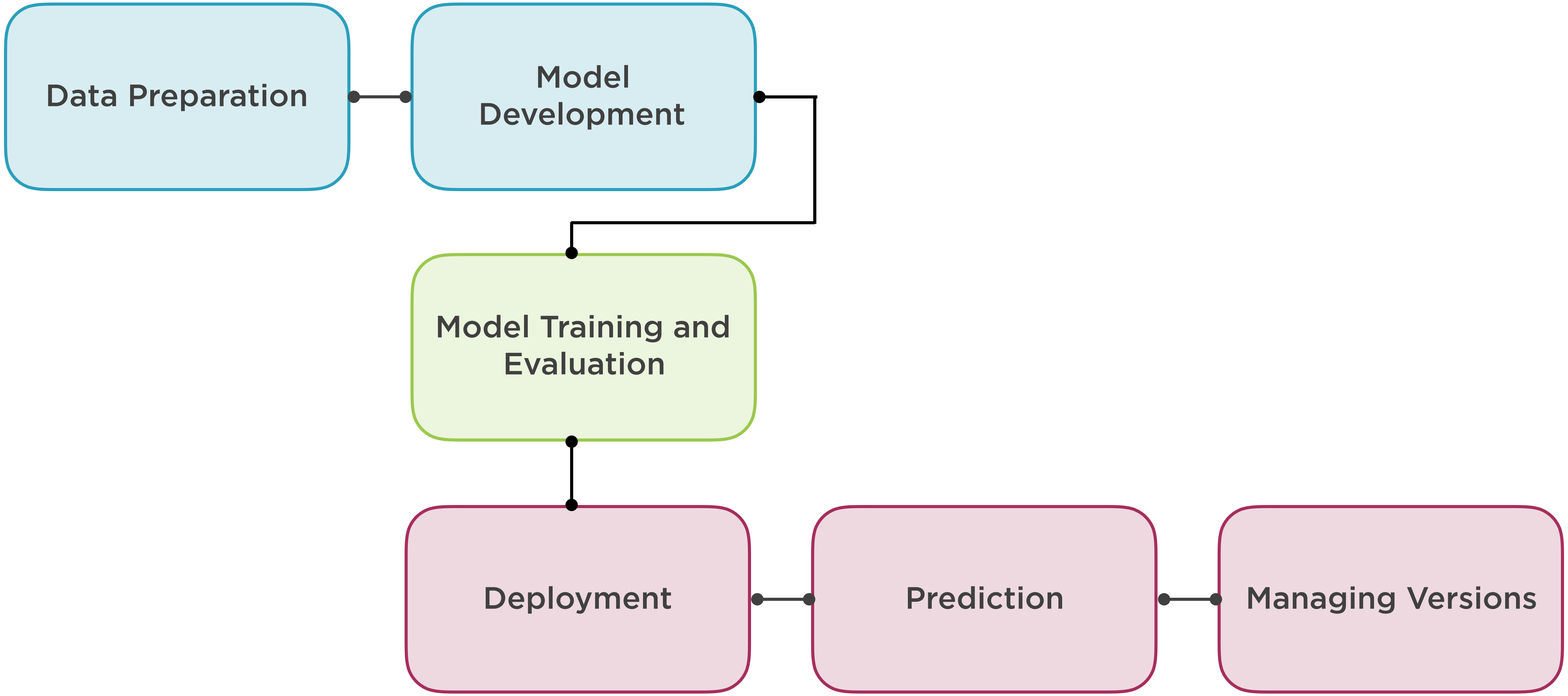


Machine Learning Workflow



TensorFlow, Keras
XGBoost and
scikit-learn

Machine Learning Workflow



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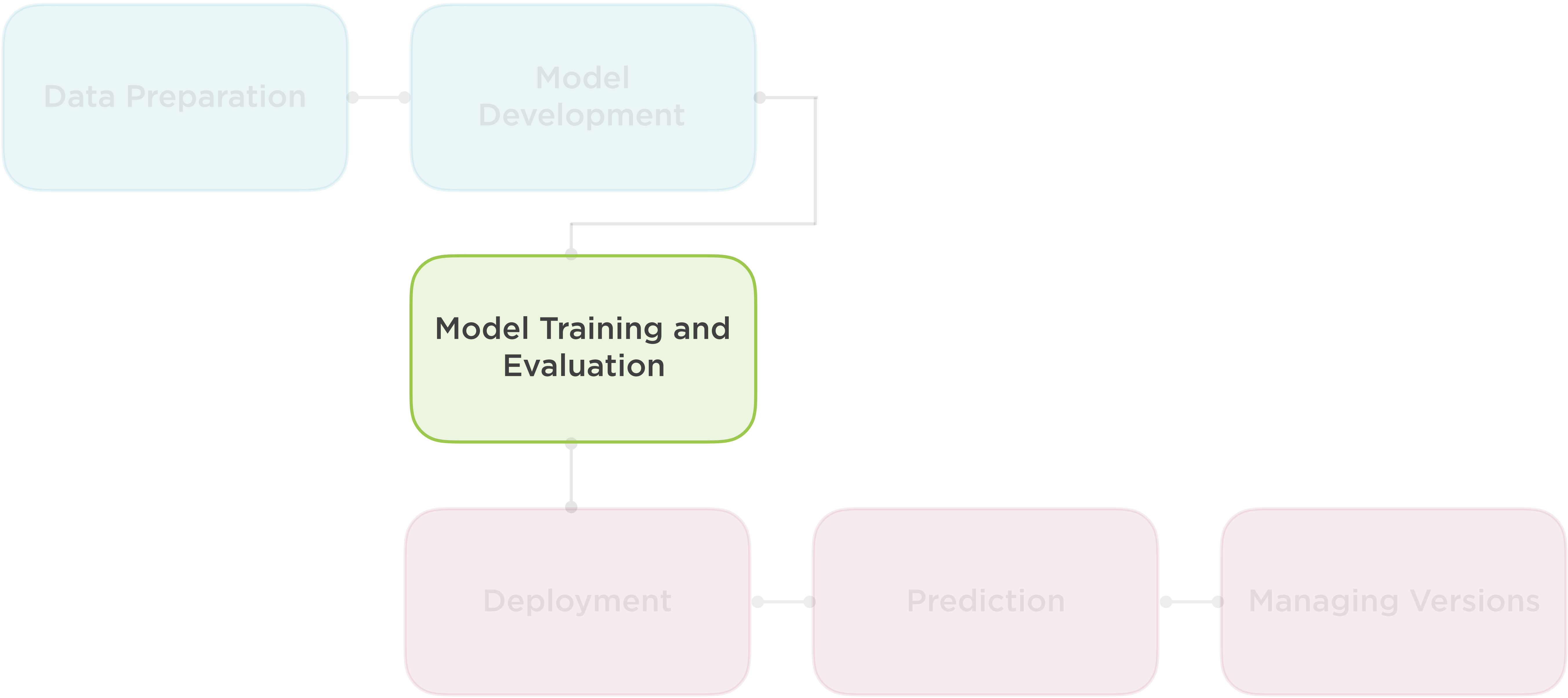
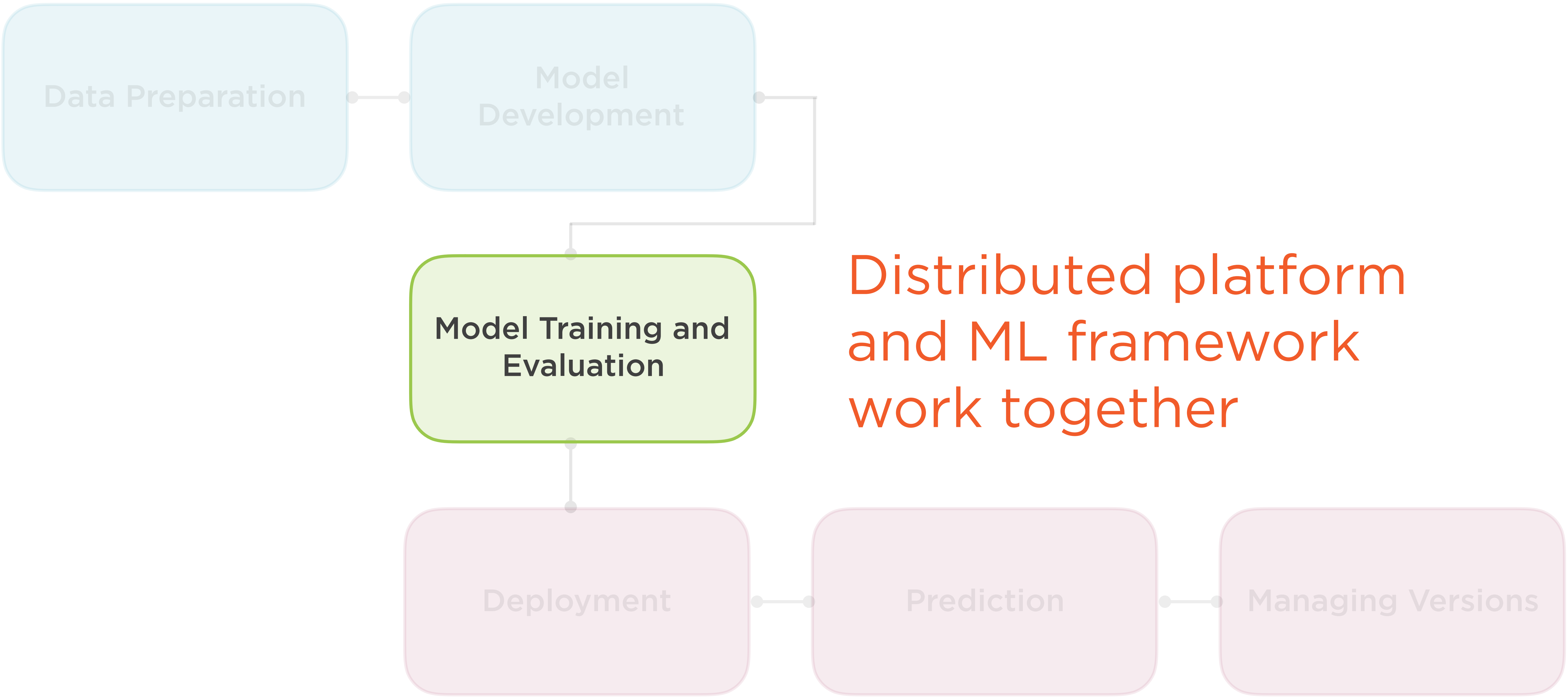
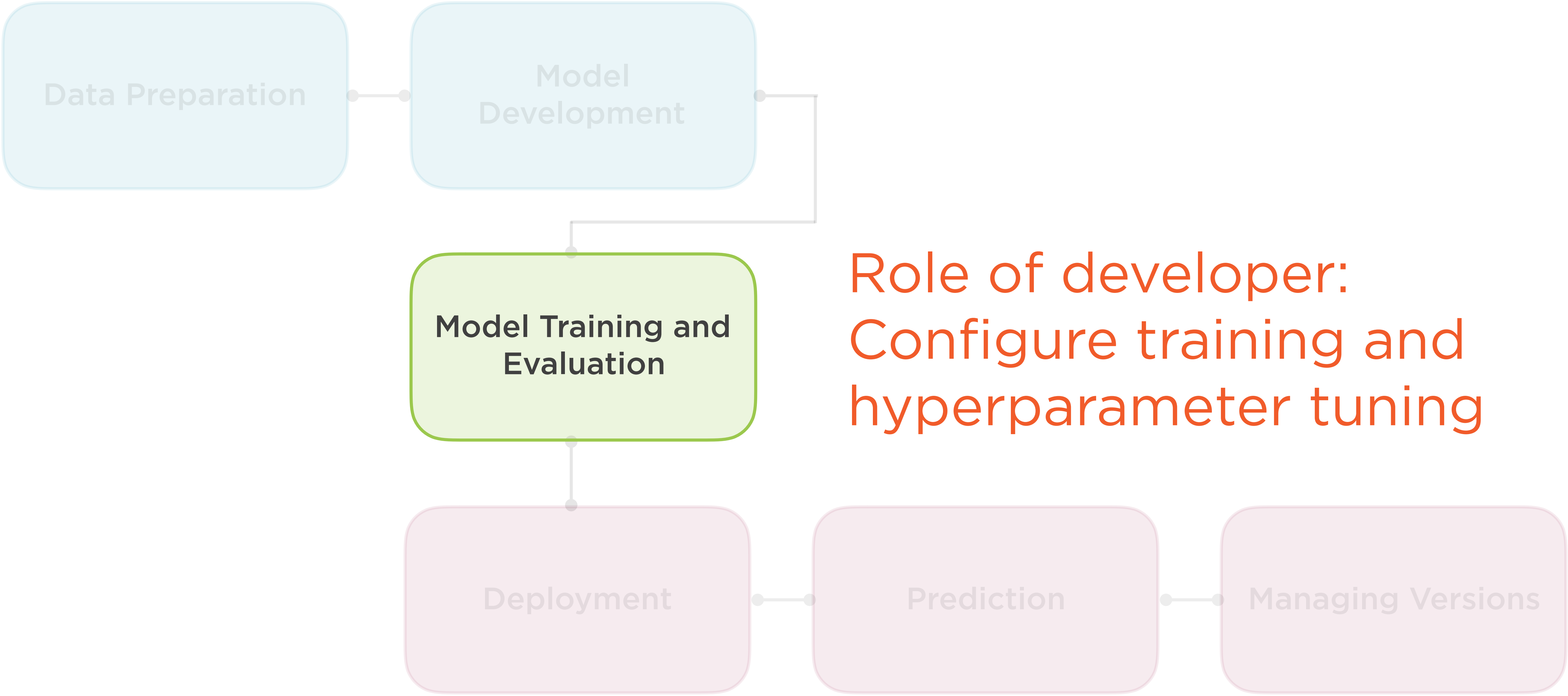


Machine Learning Workflow



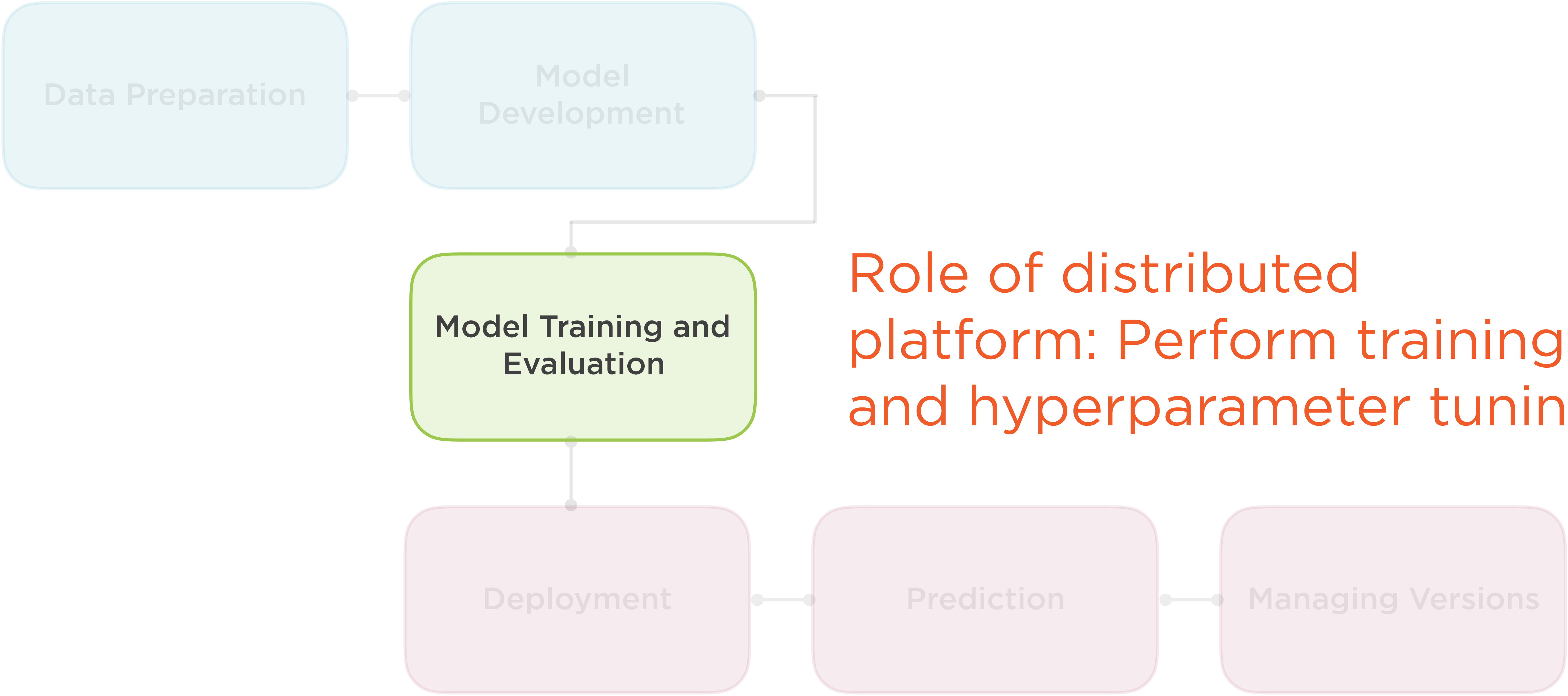
Distributed platform and ML framework work together

Machine Learning Workflow



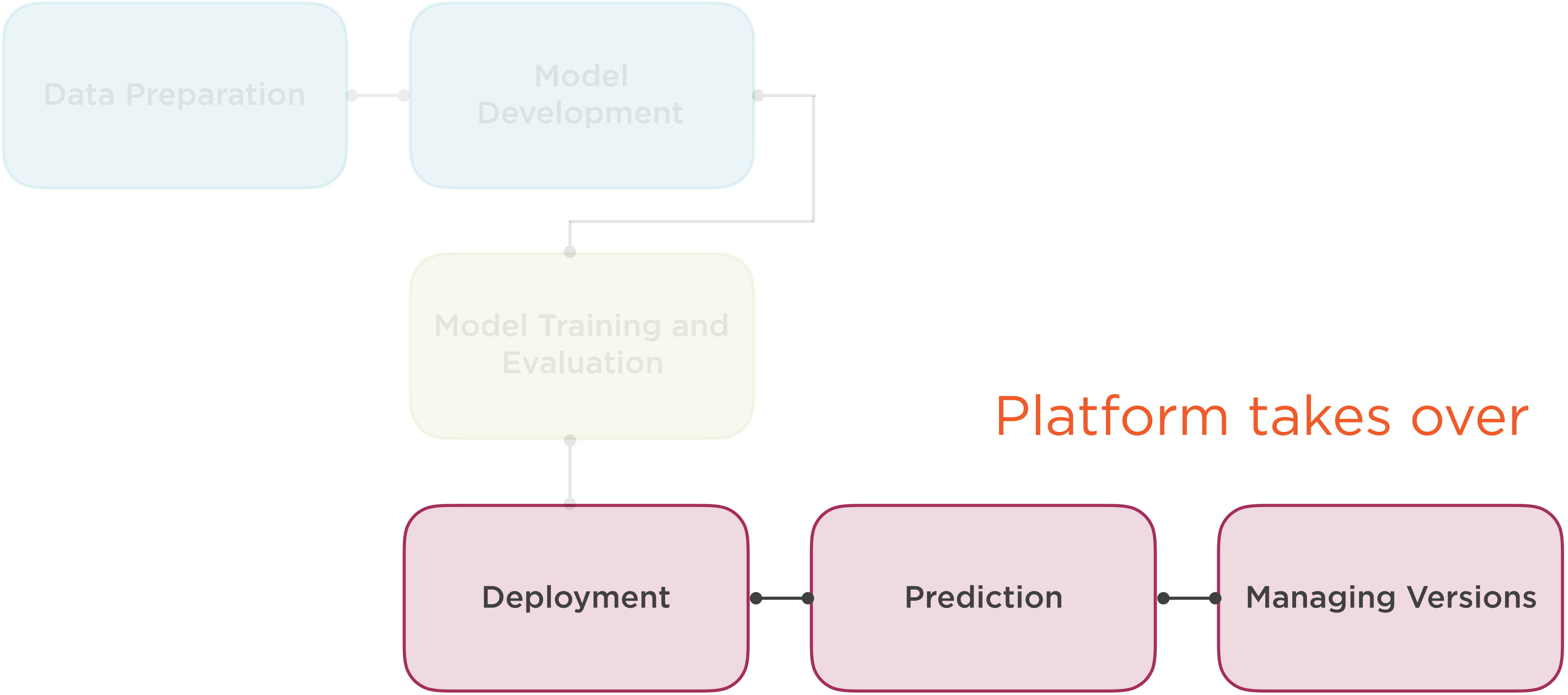
Role of developer:
Configure training and hyperparameter tuning

Machine Learning Workflow

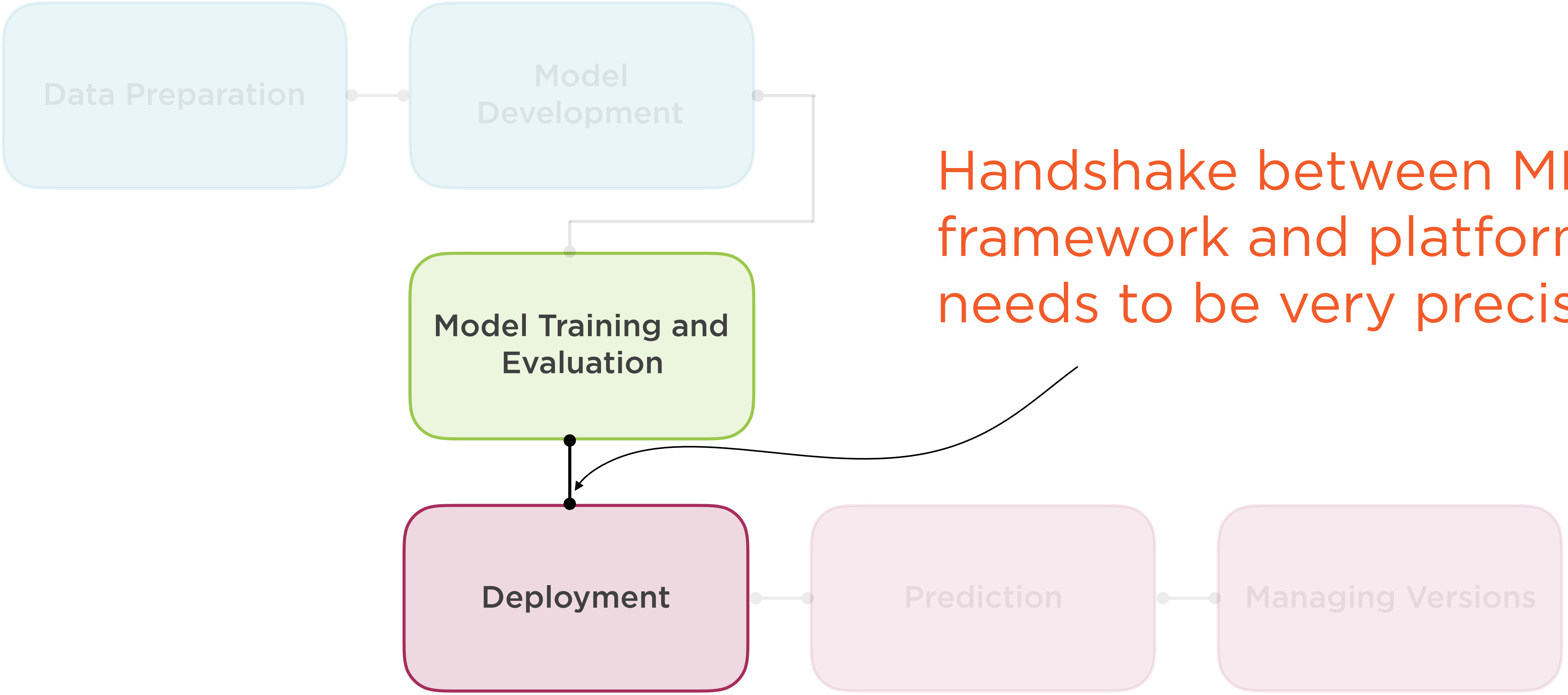


Role of distributed platform: Perform training and hyperparameter tuning

Machine Learning Workflow

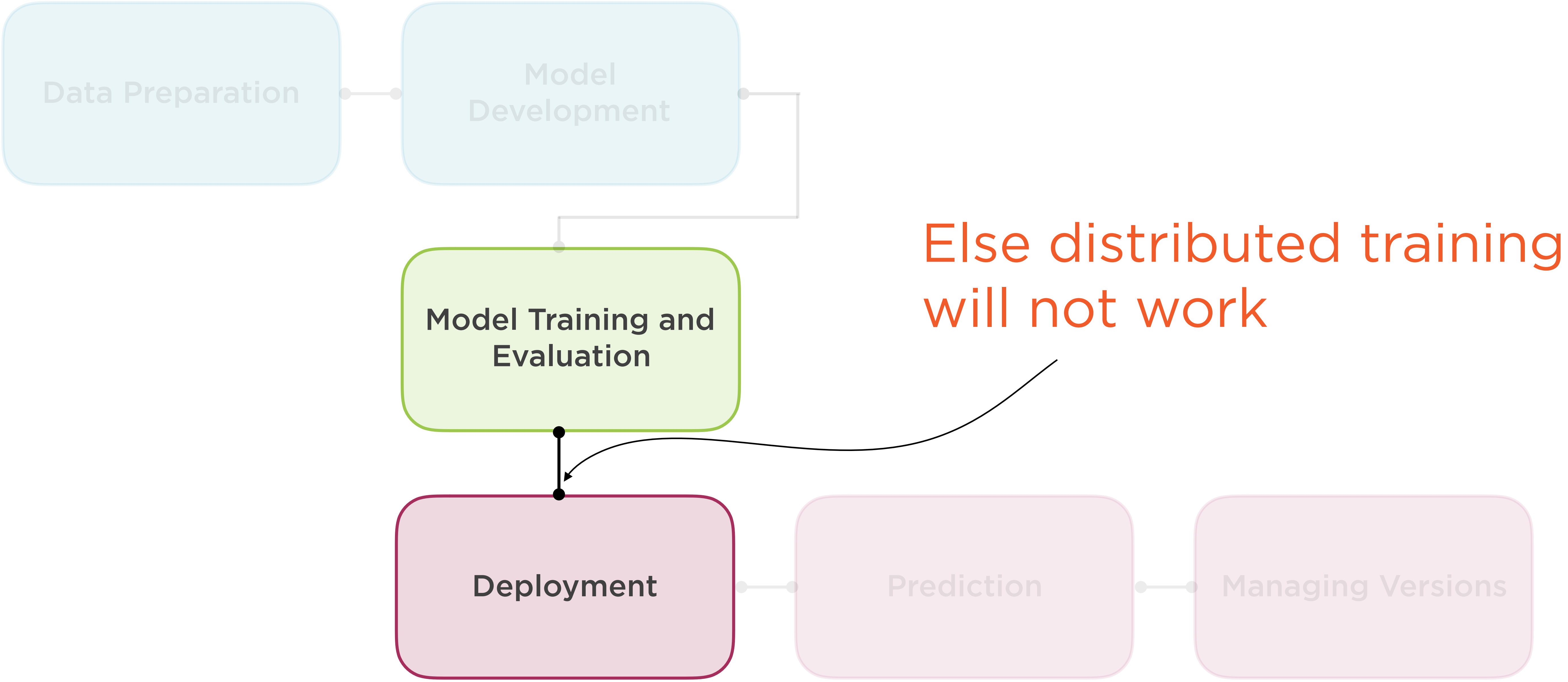


Machine Learning Workflow



Handshake between ML framework and platform needs to be very precise

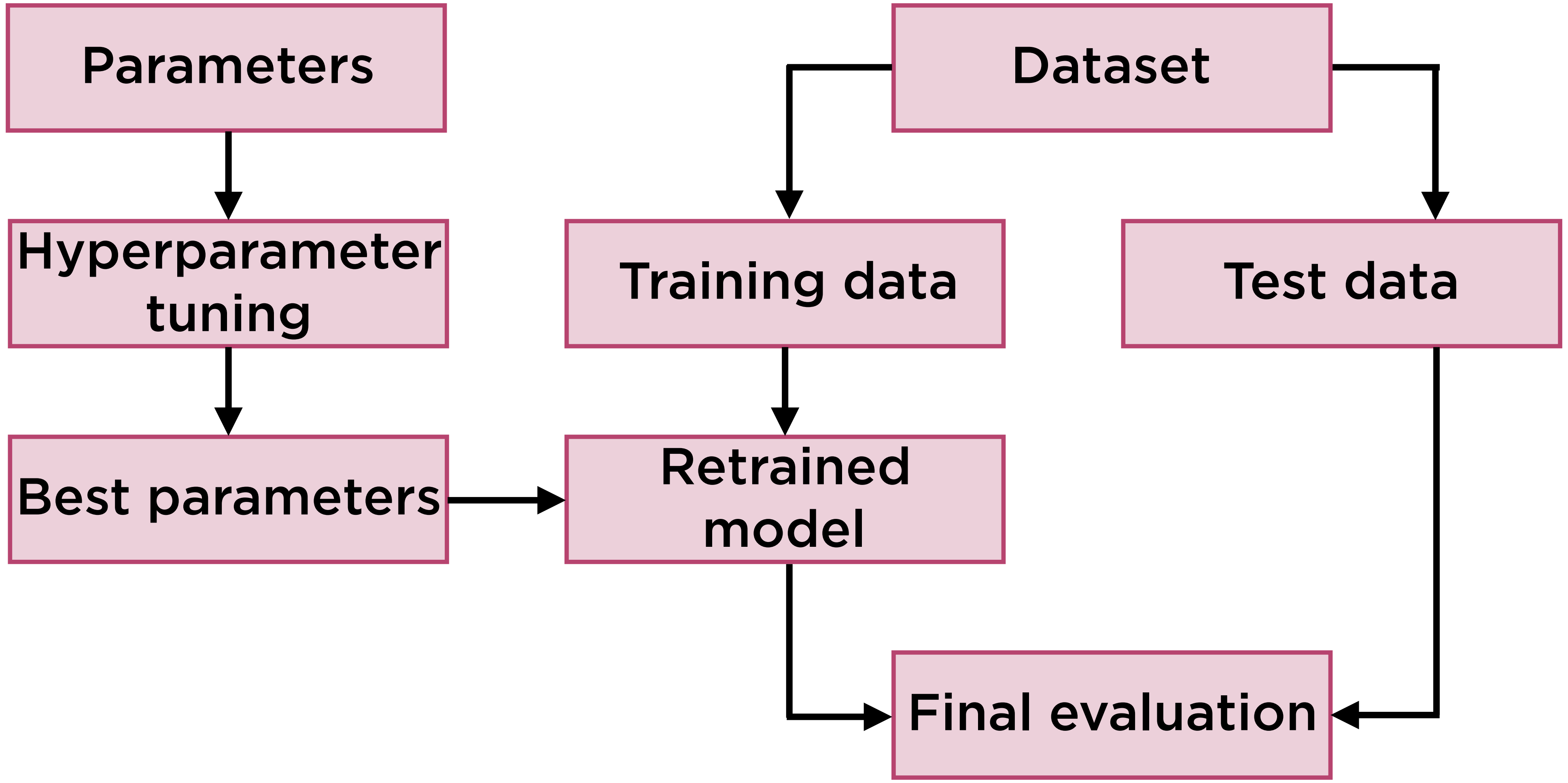
Machine Learning Workflow



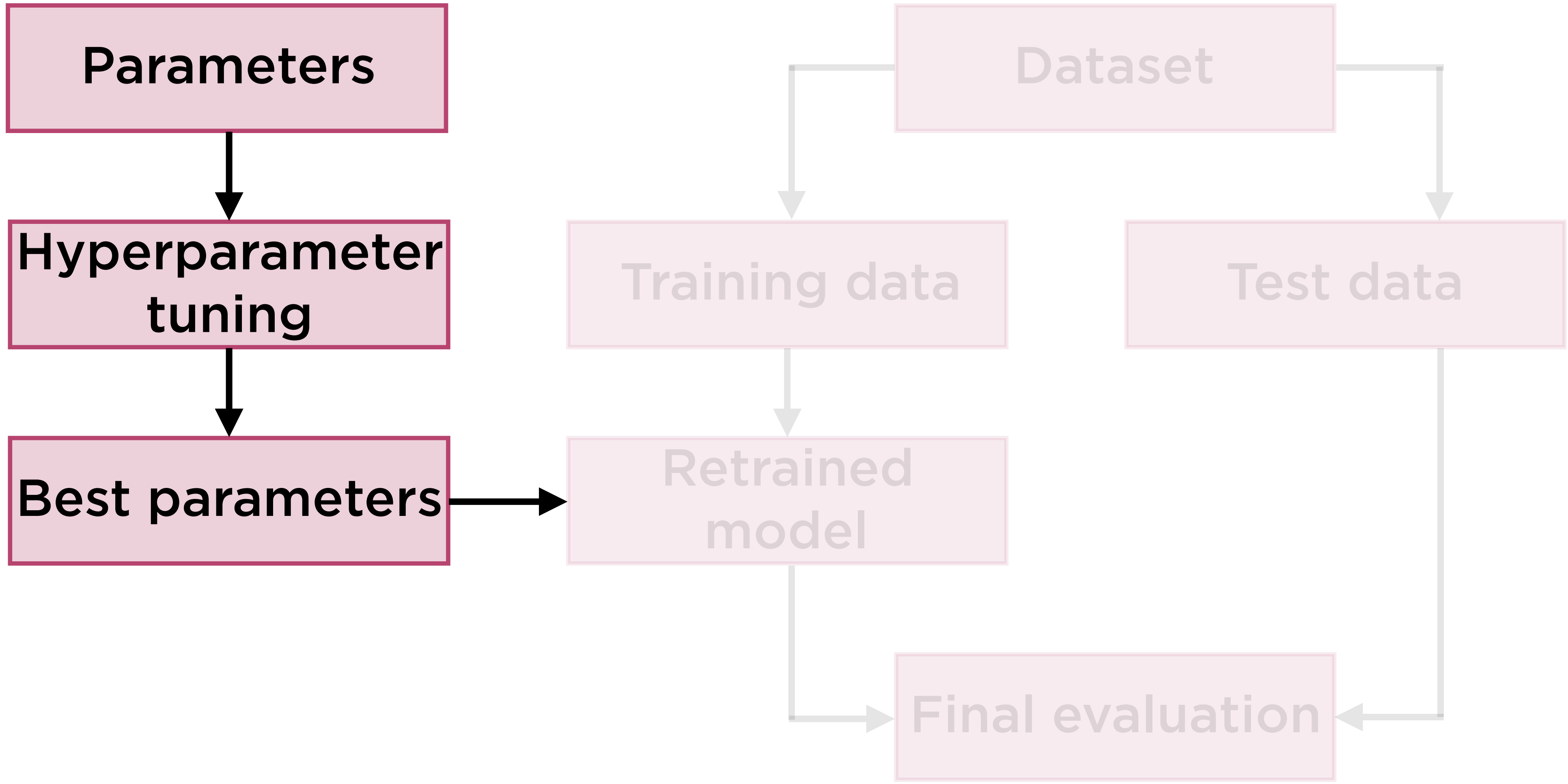
Hyperparameter tuning involves finding the best design for a model

Training involves getting the model to learn from data

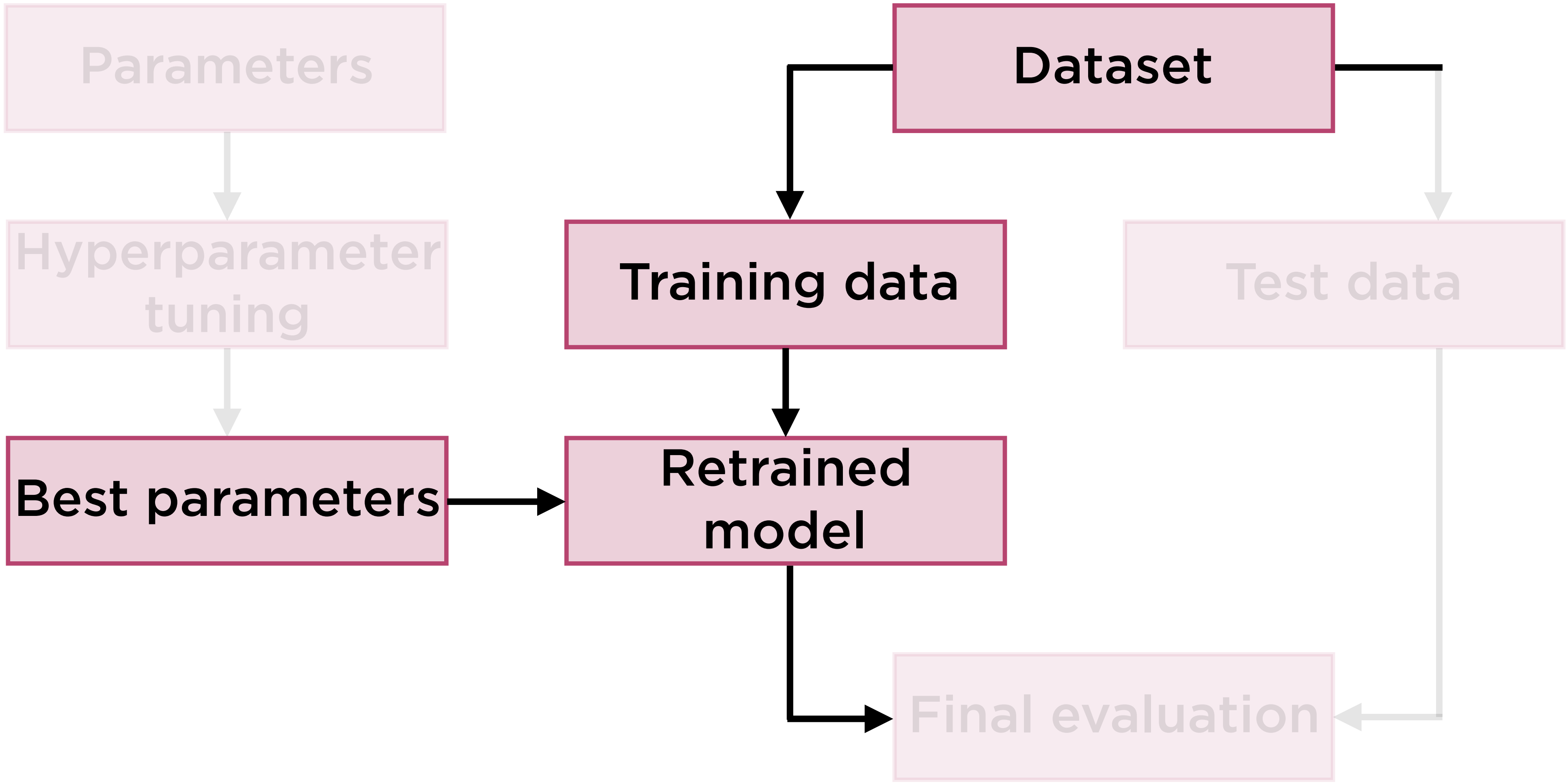
Evaluating Model Performance



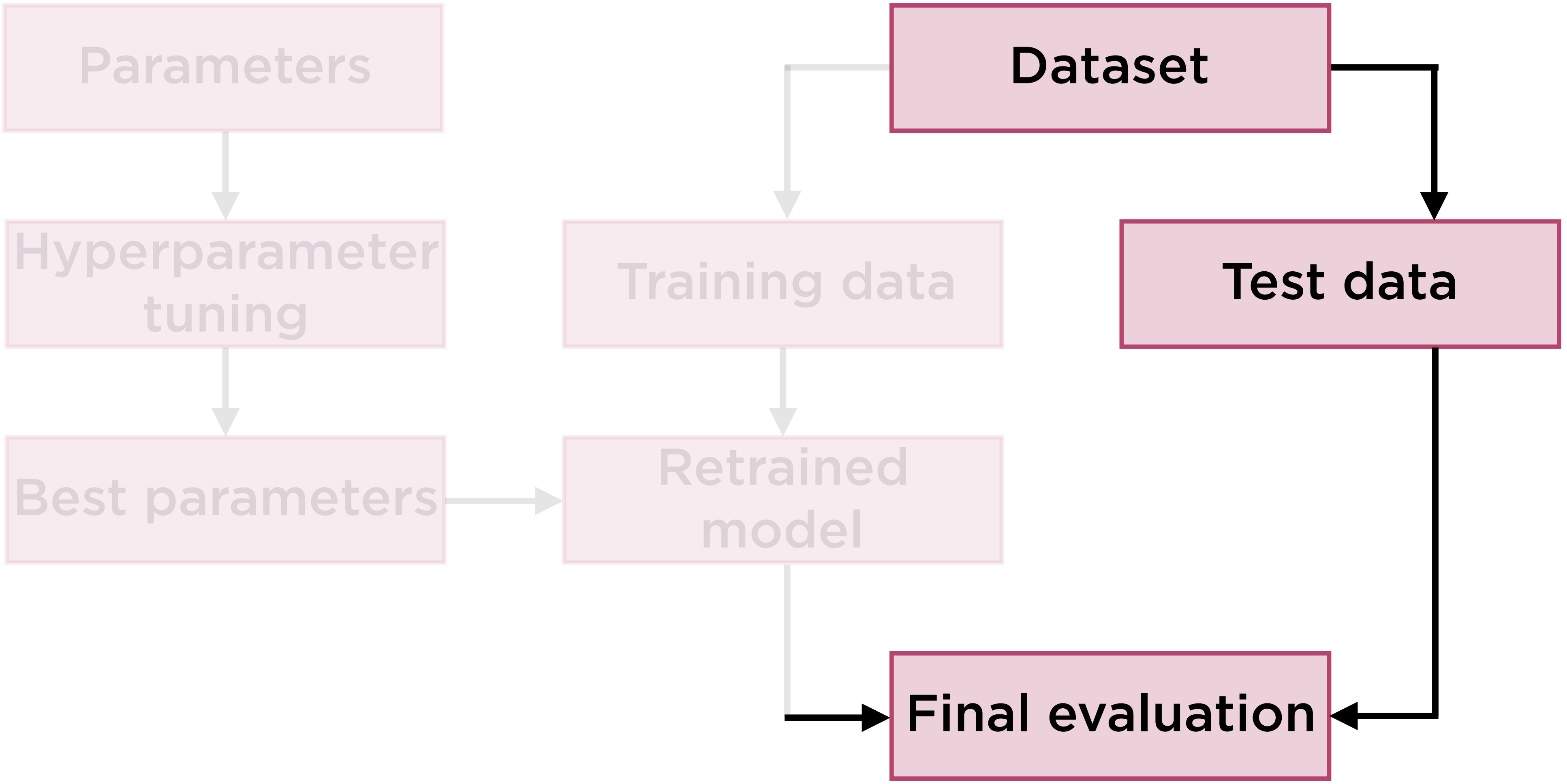
Hyperparameter Tuning to Find Best Model



Train Model with Best Design



Evaluate Model



Decision Trees

Jockey or Basketball Player?

Jockeys

Tend to be light to meet horse carrying limits

Basketball Players

Tend to be tall, strong and heavy

Jockey or Basketball Player?

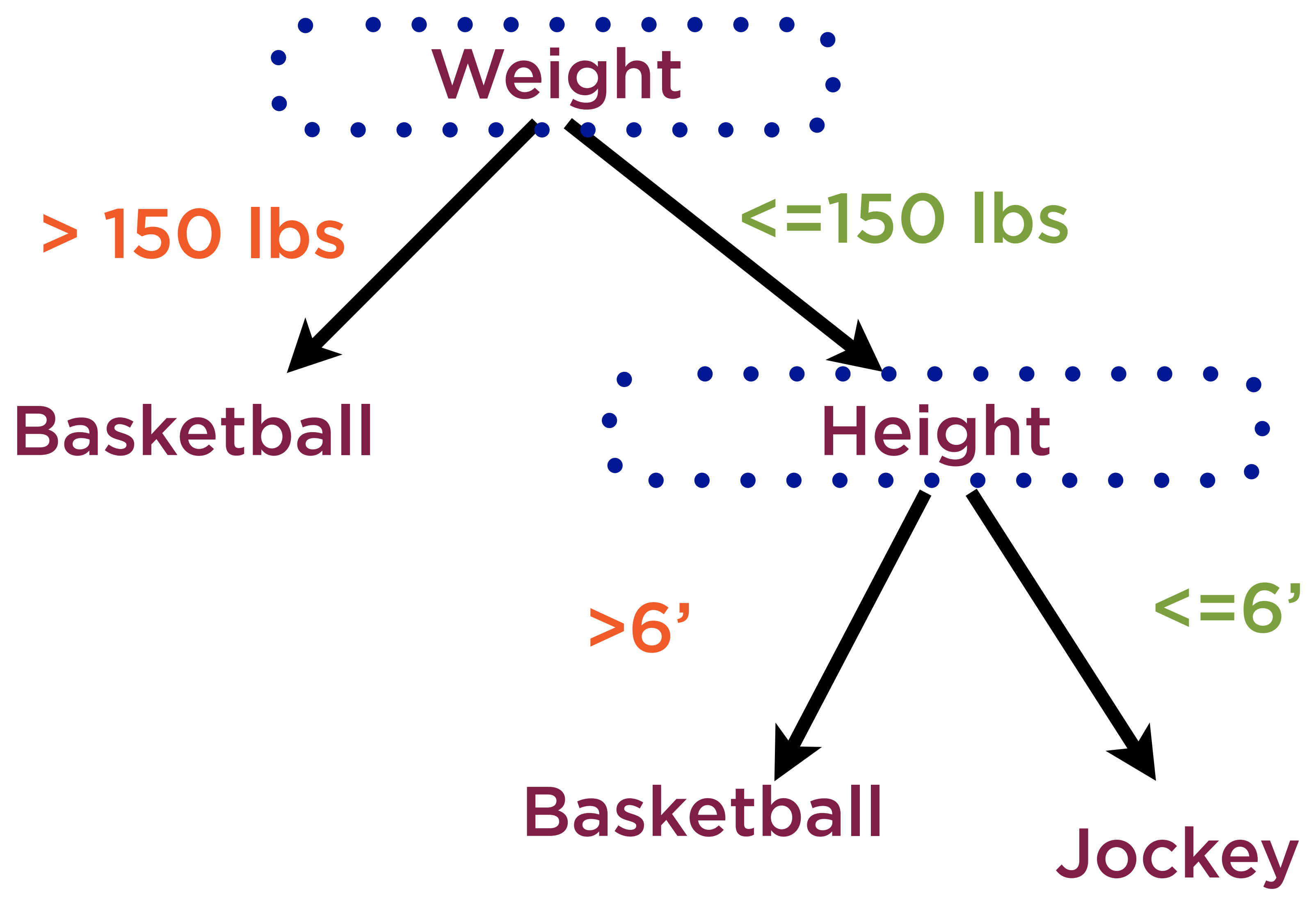
Intuitively know

- jockeys tend to be light...
- ...and not very tall
- basketball players tend to be tall
- ...and also quite heavy

Fit knowledge into rules

Each rule involves a threshold

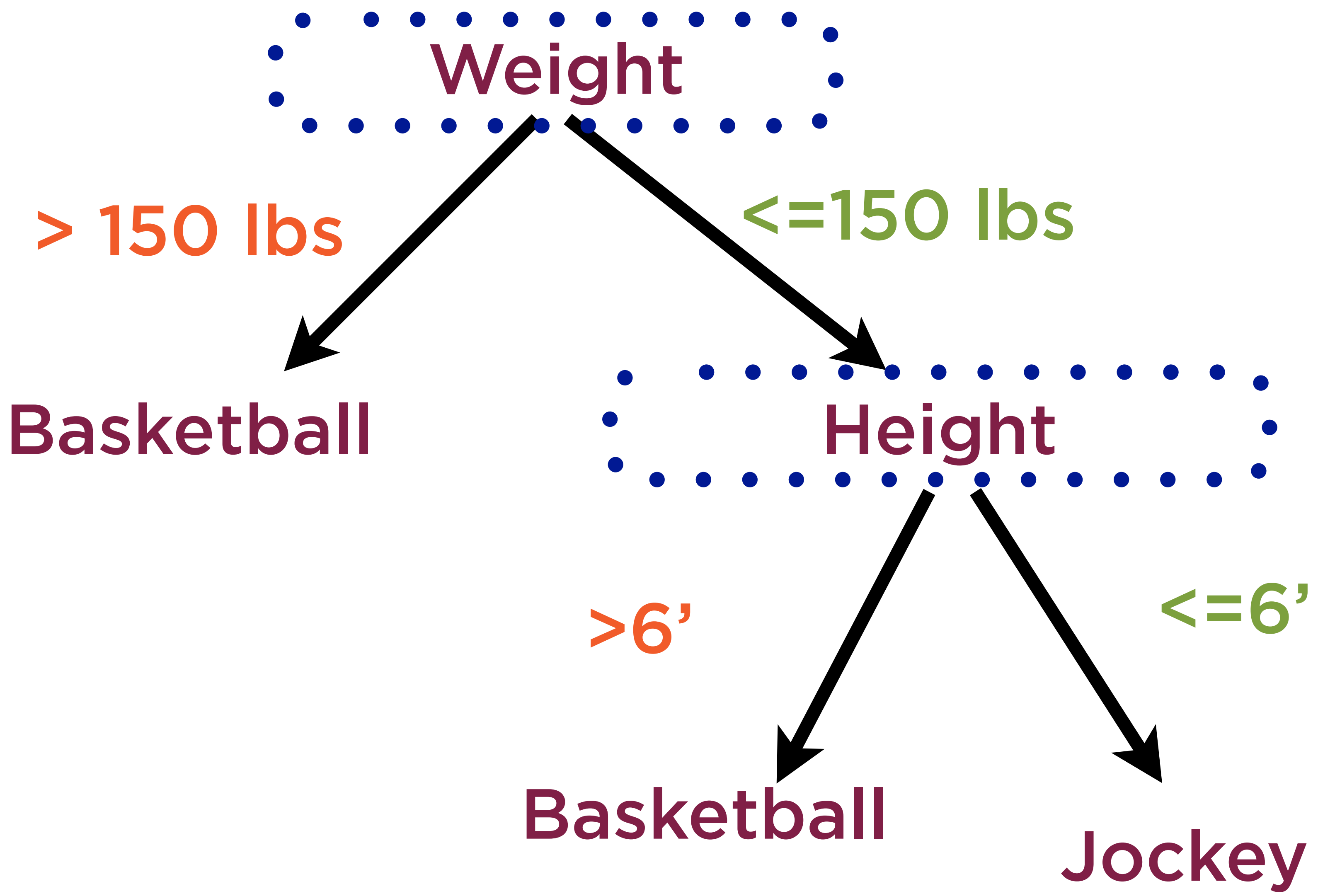
Decision Tree



Order of decision variables matters

Rules and order found using ML

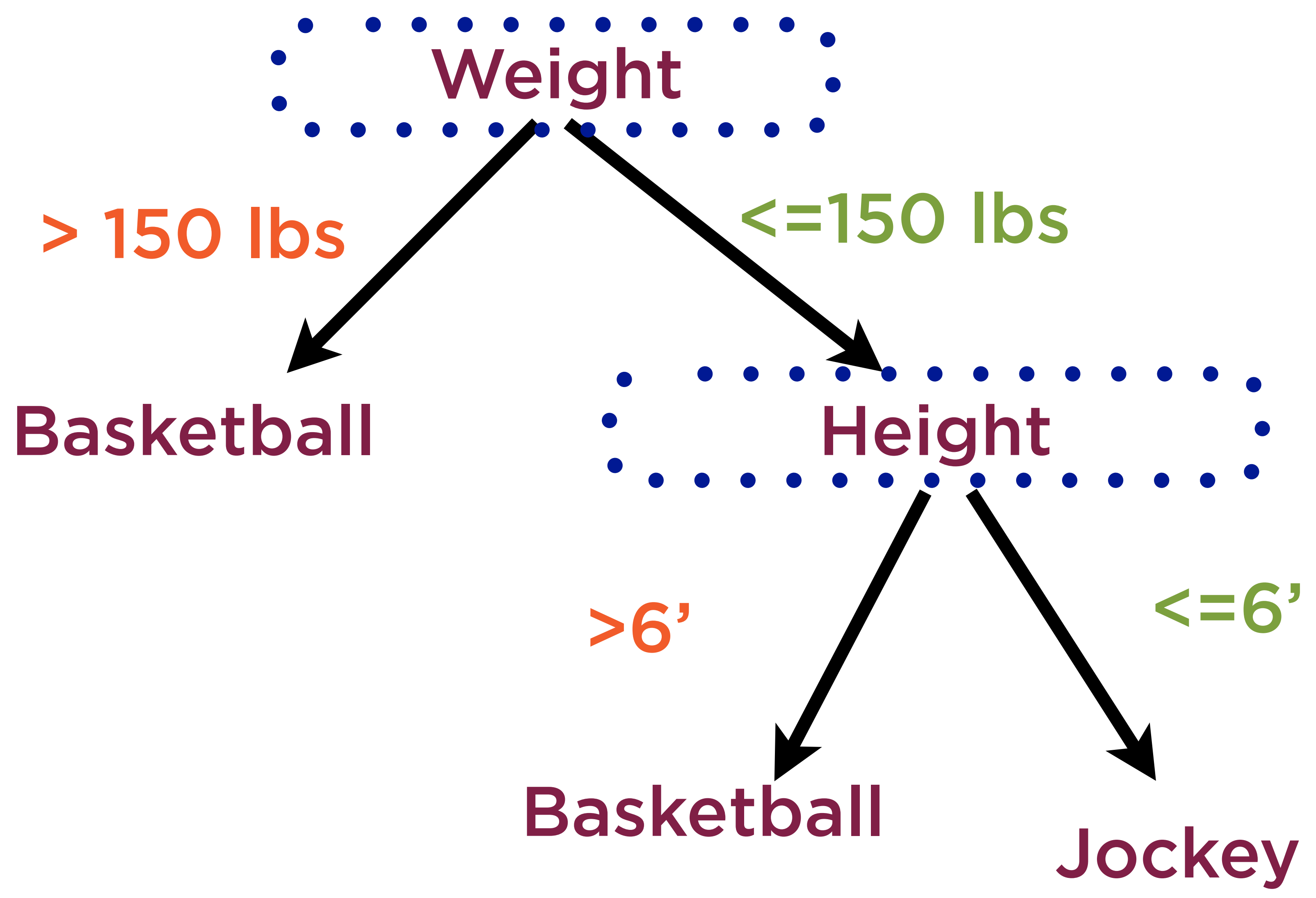
Decision Tree

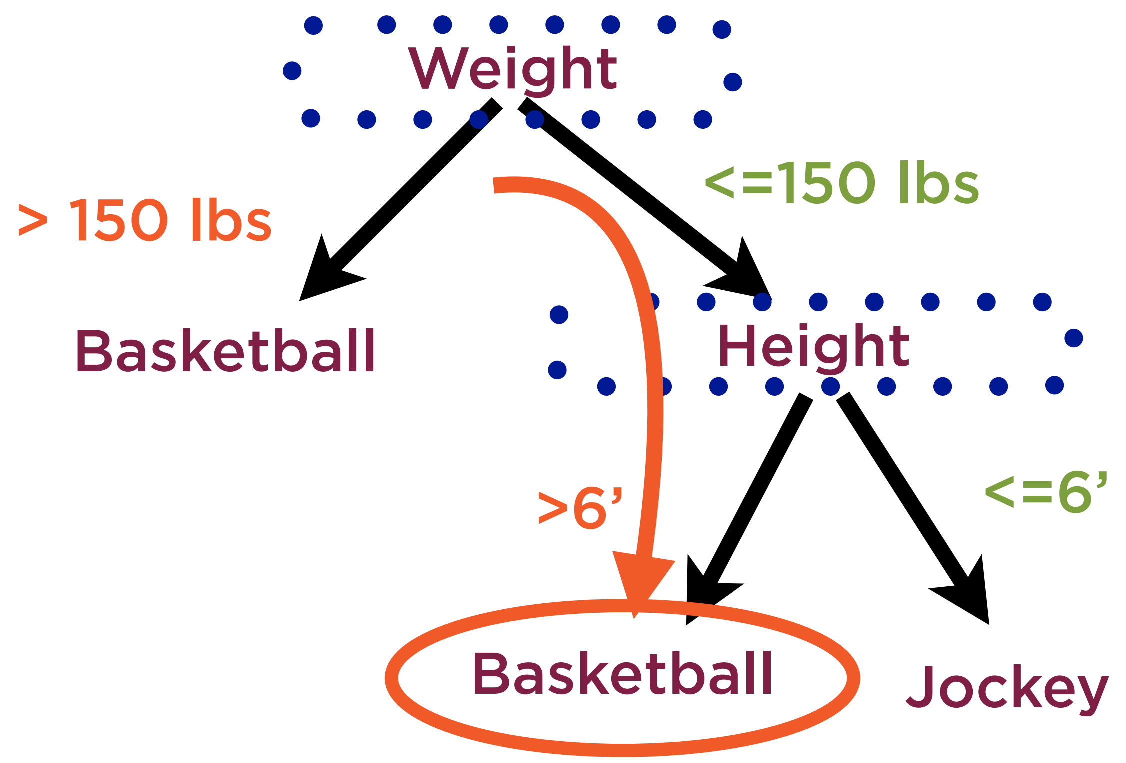


“CART”

Classification And Regression Tree

Decision Tree

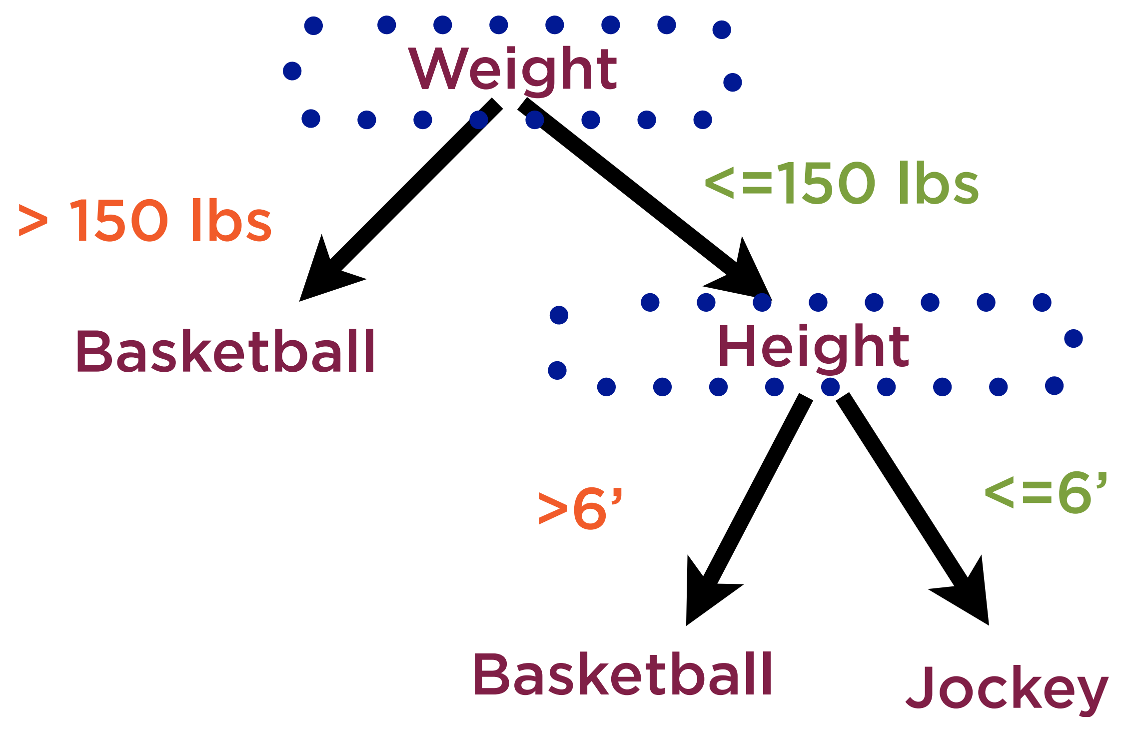




Decision Trees for Classification

To solve

- Traverse tree to find right node
- Return most frequent label of all training data points in that node

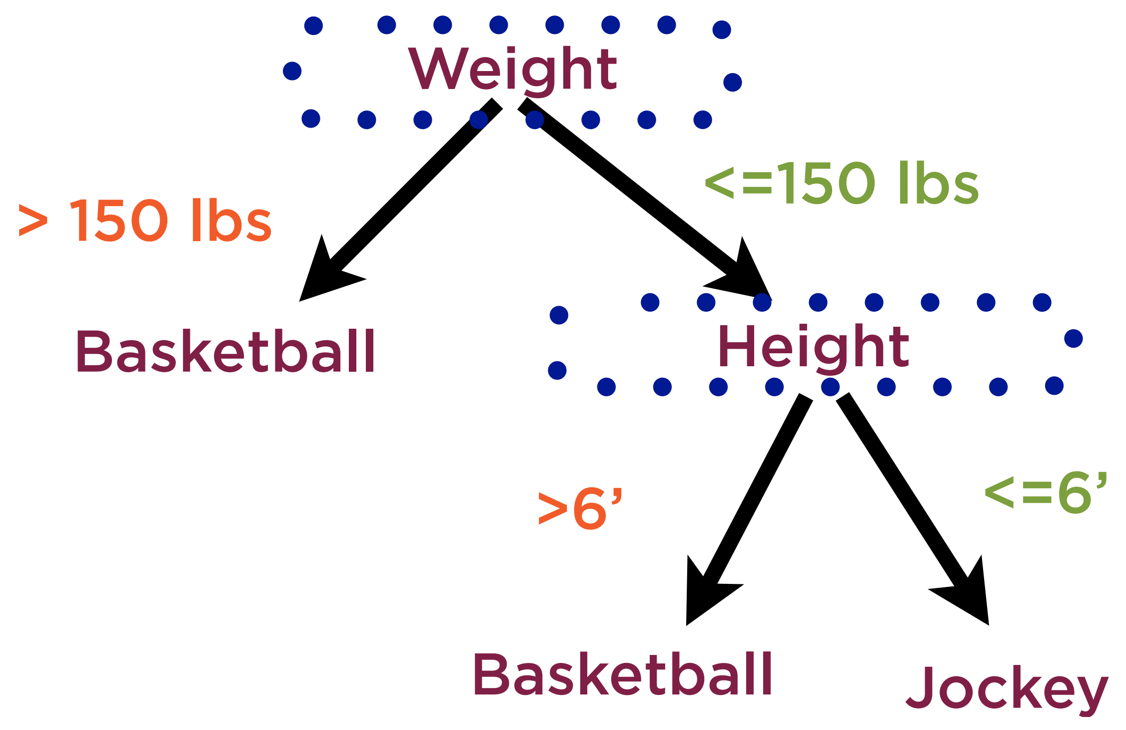


Advantages of Decision Trees

“White Box” ML ~ leverage experts

Non-parametric

- Little hyperparameter tuning
- Little data prep



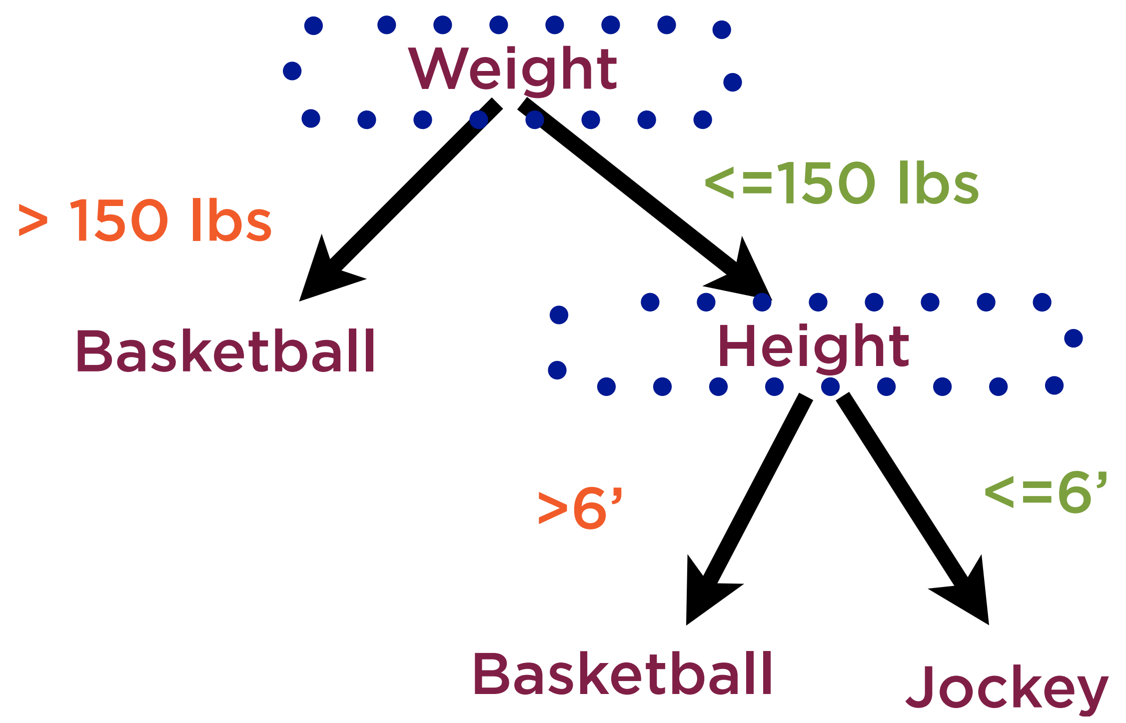
Drawbacks of Decision Trees

Prone to overfitting

- Common risk with non-parametric

Unstable

- Small changes in data cause big changes in model



Random Forests

Extremely powerful technique

Example of ensemble learning

Individual trees should be as different as possible

Hyperparameters in Decision Trees

Splitting strategy	Max depth	Min samples split
Min samples leaf	Min weight fraction	Max features

Titlecase

splitter : *string, optional (default="best")*

The strategy used to choose the split at each node. Supported strategies are "best" to choose the best split and "random" to choose the best random split.

max_depth : *int or None, optional (default=None)*

The maximum depth of the tree. If None, then nodes are expanded until all leaves are pure or until all leaves contain less than min_samples_split samples.

min_samples_split : *int, float, optional (default=2)*

The minimum number of samples required to split an internal node:

- If int, then consider `min_samples_split` as the minimum number.
- If float, then `min_samples_split` is a fraction and `ceil(min_samples_split * n_samples)` are the minimum number of samples for each split.

Changed in version 0.18: Added float values for fractions.

min_samples_leaf : *int, float, optional (default=1)*

The minimum number of samples required to be at a leaf node. A split point at any depth will only be considered if it leaves at least `min_samples_leaf` training samples in each of the left and right branches. This may have the effect of smoothing the model, especially in regression.

- If int, then consider `min_samples_leaf` as the minimum number.
- If float, then `min_samples_leaf` is a fraction and `ceil(min_samples_leaf * n_samples)` are the minimum number of samples for each node.

Changed in version 0.18: Added float values for fractions.

min_weight_fraction_leaf : ***float, optional (default=0.)***

The minimum weighted fraction of the sum total of weights (of all the input samples) required to be at a leaf node. Samples have equal weight when sample_weight is not provided.

max_features : ***int, float, string or None, optional (default=None)***

The number of features to consider when looking for the best split:

- If int, then consider `max_features` features at each split.
- If float, then `max_features` is a fraction and `int(max_features * n_features)` features are considered at each split.
- If "auto", then `max_features=sqrt(n_features)`.
- If "sqrt", then `max_features=sqrt(n_features)`.
- If "log2", then `max_features=log2(n_features)`.
- If None, then `max_features=n_features`.

Note: the search for a split does not stop until at least one valid partition of the node samples is found, even if it requires to effectively inspect more than `max_features` features.

random_state : *int, RandomState instance or None, optional (default=None)*

If int, random_state is the seed used by the random number generator; If RandomState instance, random_state is the random number generator; If None, the random number generator is the RandomState instance used by `np.random`.

max_leaf_nodes : *int or None, optional (default=None)*

Grow a tree with `max_leaf_nodes` in best-first fashion. Best nodes are defined as relative reduction in impurity. If None then unlimited number of leaf nodes.

min_impurity_decrease : *float, optional (default=0.)*

A node will be split if this split induces a decrease of the impurity greater than or equal to this value.

The weighted impurity decrease equation is the following:

```
N_t / N * (impurity - N_t_R / N_t * right_impurity
                    - N_t_L / N_t * left_impurity)
```

where `N` is the total number of samples, `N_t` is the number of samples at the current node, `N_t_L` is the number of samples in the left child, and `N_t_R` is the number of samples in the right child.

`N`, `N_t`, `N_t_R` and `N_t_L` all refer to the weighted sum, if `sample_weight` is passed.

New in version 0.19.

min_impurity_split : *float, (default=1e-7)*

Threshold for early stopping in tree growth. A node will split if its impurity is above the threshold, otherwise it is a leaf.

Deprecated since version 0.19: `min_impurity_split` has been deprecated in favor of `min_impurity_decrease` in 0.19. The default value of `min_impurity_split` will change from 1e-7 to 0 in 0.23 and it will be removed in 0.25. Use `min_impurity_decrease` instead.

Demo

Hyperparameter tuning using Azure ML Studio

Summary

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