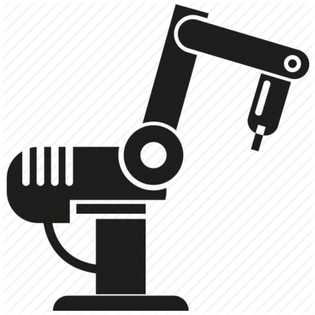
Scalable Automatic Machine Learning in H2O



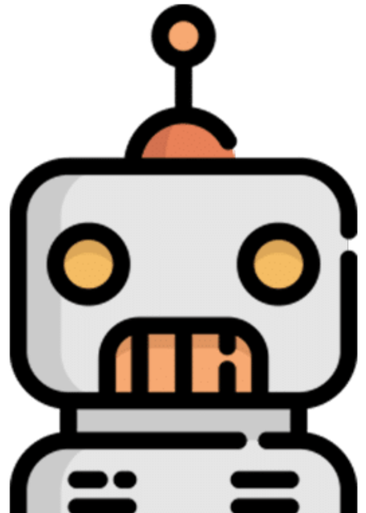
May 2018
2018 Symposium on Data Science and Statistics

H2O.ai

Navdeep Gill
@Navdeep_Gill_

Agenda

- H2O Platform
- Automatic Machine Learning (AutoML)
- H2O AutoML Overview
- AutoML Pro Tips
- Demos



Company Overview

Founded	2011 Venture-backed, Debuted in 2012
Products	• **H_2O Open Source In-Memory AI Prediction Engine** • Sparkling Water (H_2O + Spark) • H2O4GPU (H2O on GPUs) • Enterprise Steam • Driverless AI
Mission	Operationalize Data Science & Provide a Platform to Build Beautiful Data Products
Team	75+ employees • Distributed Systems Engineers doing Machine Learning • World-class Visualization Designers
Headquarters	Mountain View, CA

Scientific Advisory Council

Dr. Trevor Hastie

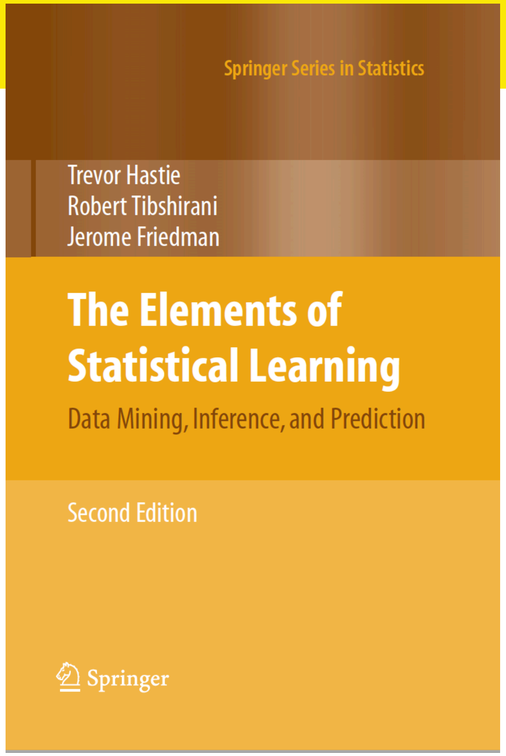
- PhD in Statistics, Stanford University
- John A. Overdeck Professor of Mathematics, Stanford University
- Co-author, *The Elements of Statistical Learning: Prediction, Inference and Data Mining*
- Co-author, *Generalized Additive Models*
- 108,404 citations (via Google Scholar)

Dr. Robert Tibshirani

- PhD in Statistics, Stanford University
- Professor of Statistics and Health Research and Policy, Stanford University
- COPPS Presidents' Award recipient
- Co-author, *The Elements of Statistical Learning: Prediction, Inference and Data Mining*
- Author, *Regression Shrinkage and Selection via the Lasso*
- Co-author, *An Introduction to the Bootstrap*

Dr. Steven Boyd

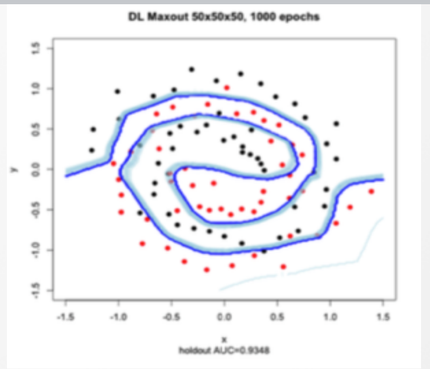
- PhD in Electrical Engineering and Computer Science, UC Berkeley
- Professor of Electrical Engineering and Computer Science, Stanford University
- Co-author, Convex Optimization
- Co-author, Linear Matrix Inequalities in System and Control Theory
- Co-author, *Distributed Optimization and Statistical Learning via the Alternating Direction Method of Multipliers*



H2O.ai

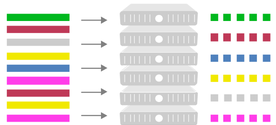
What is H2O?

Java-Based Software for **In-Memory** **Data Modeling**

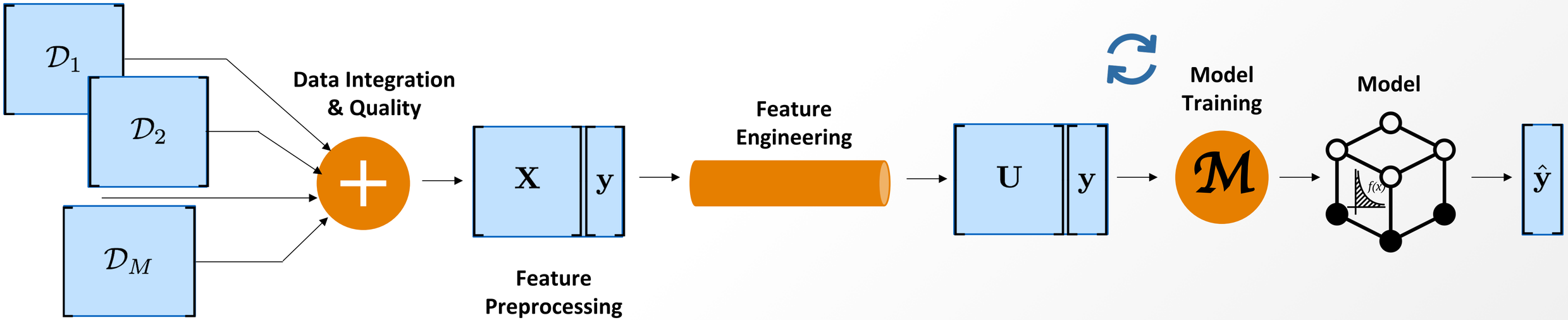
Open Source	Big Data Ecosystem	Flexible Interface	Smart and Fast Algorithms
			

What is H2O?

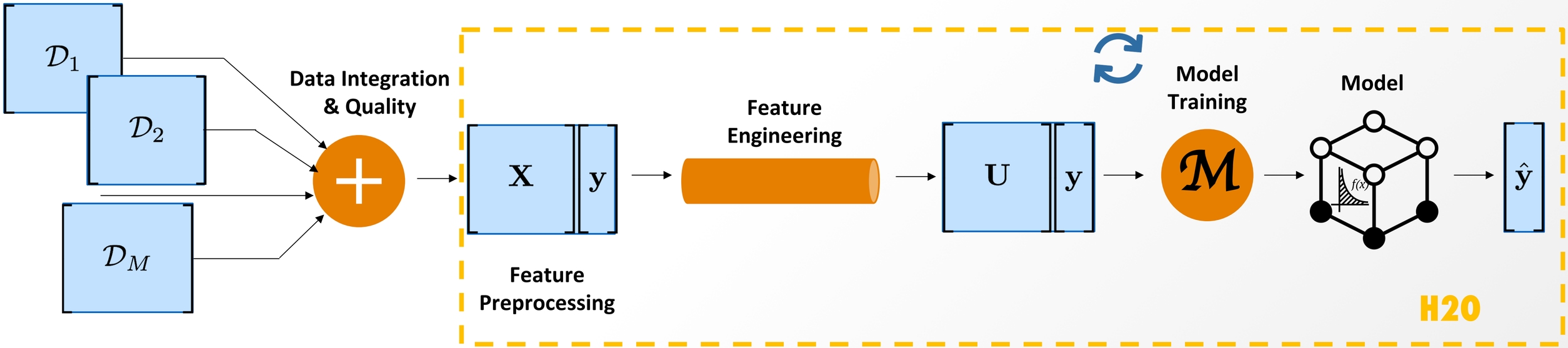
Java-Based Software for **In-Memory** **Data Modeling**

Scalability and Performance	Rapid Model Deployment	GPU Enablement*	Cloud Integration
	• Highly portable models deployed in Java (POJO) • Automated and streamlined scoring service deployment with Rest API*		  
• Distributed In-Memory Computing Platform • Distributed Algorithms • Fine-Grain MapReduce			

The Machine Learning Pipeline



Where H2O Fits



Current Algorithm Overview

Statistical Analysis

- Linear Models (GLM)
- Naïve Bayes

Ensembles

- Random Forest
- Gradient Boosting Machine
- Stacking / Super Learner

Deep Neural Networks

- MLP
- Autoencoder
  - Anomaly Detection
  - Deep Features

Clustering

- K-Means (Auto-*K*)

Dimension Reduction

- Principal Component Analysis
- Generalized Low Rank Models

Word Embedding

- Word2Vec

Time Series

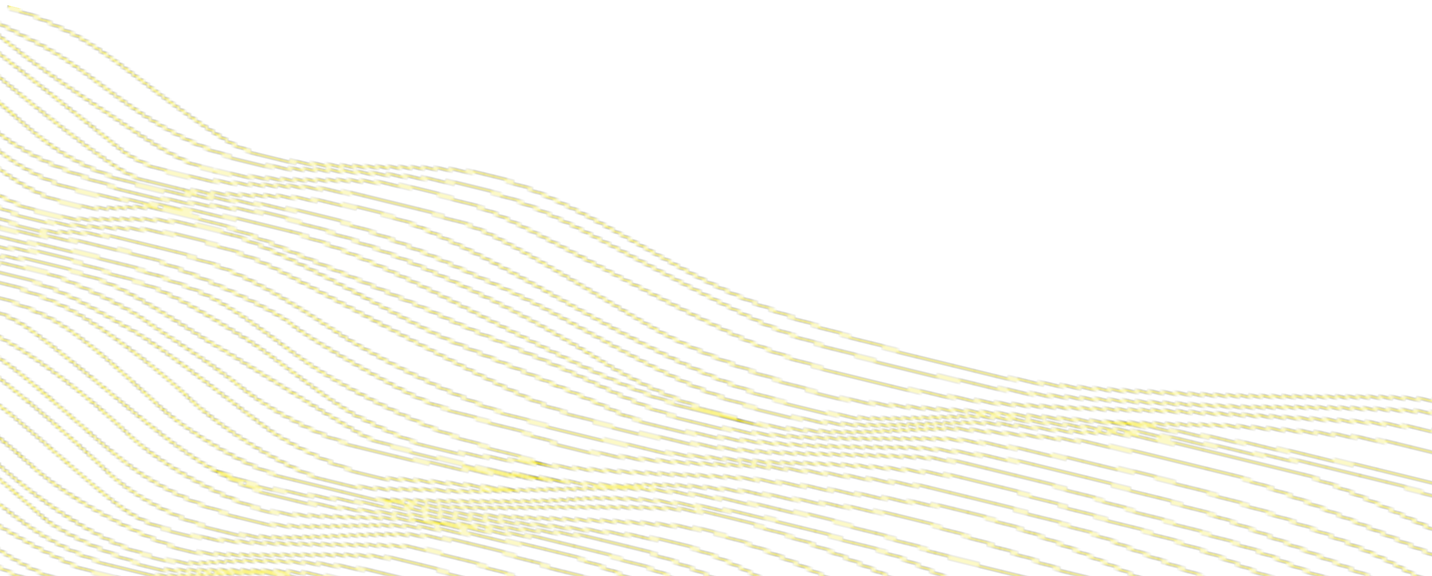
- iSAX

Machine Learning Tuning

- Hyperparameter Search
- Early Stopping

H2O Core

Behind the Scenes



How H2O Core Works

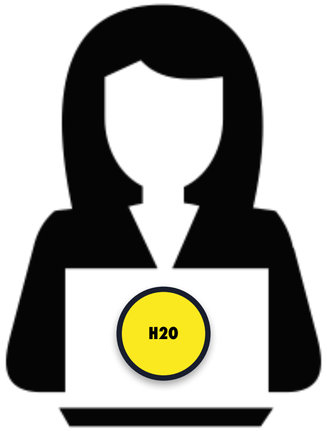
H2O

How H2O Core Works

(just a java application)

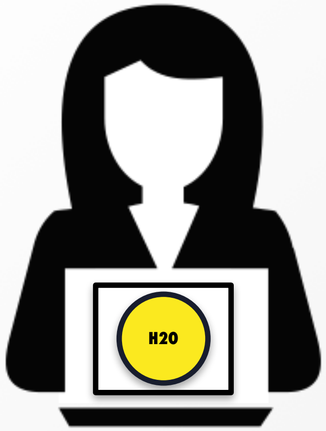
How H2O Core Works

How H2O Core Works



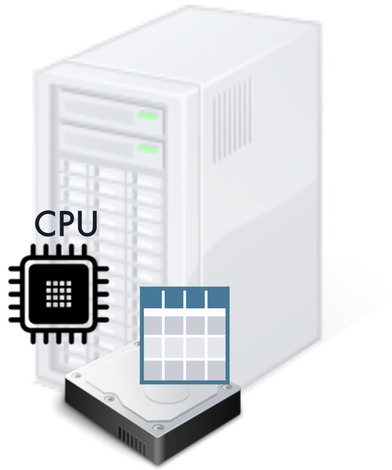
on a laptop

on a virtual machine

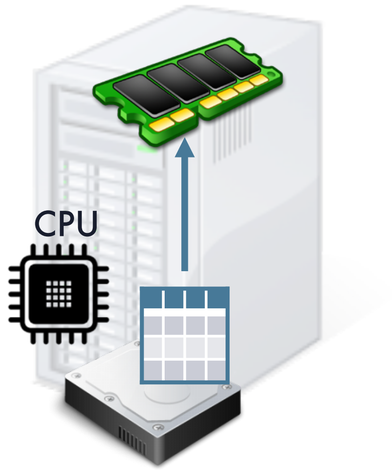


in a container

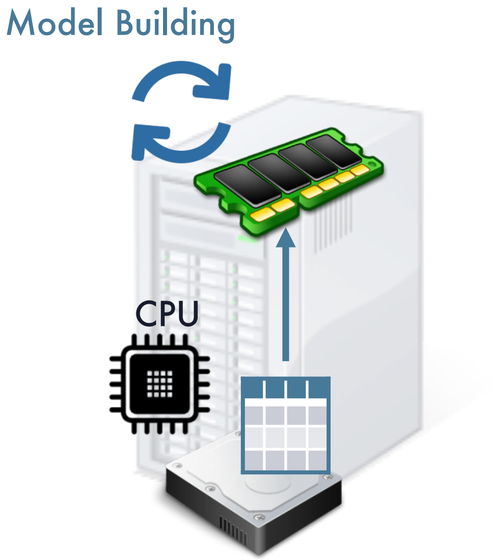
H2O Core



H2O Core



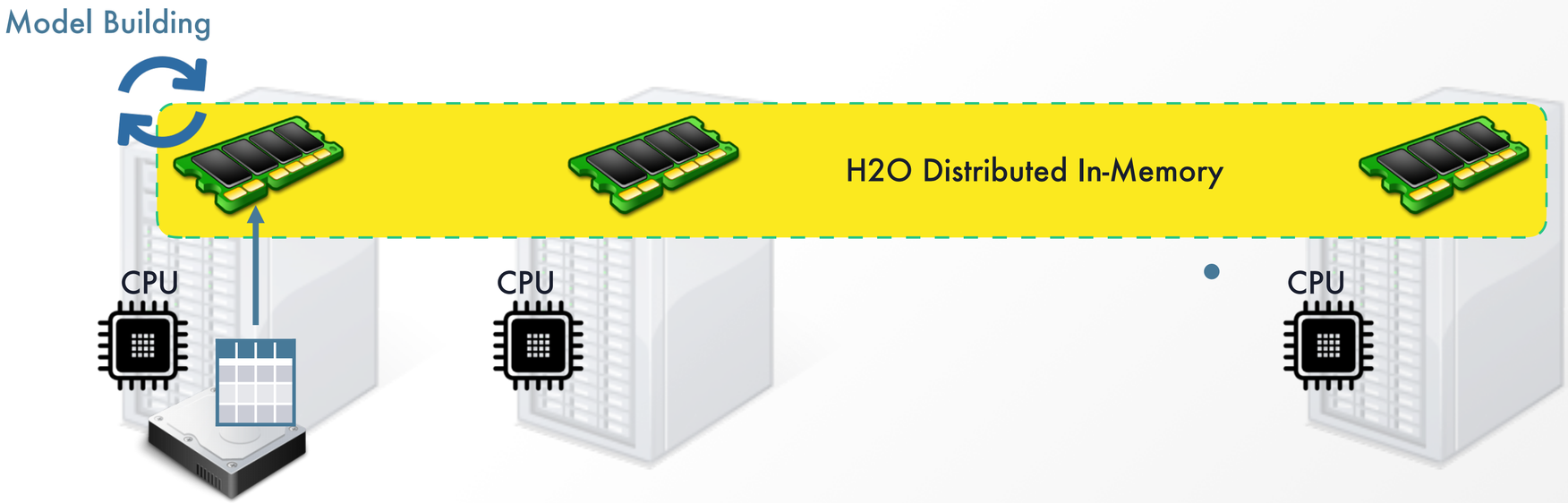
H2O Core



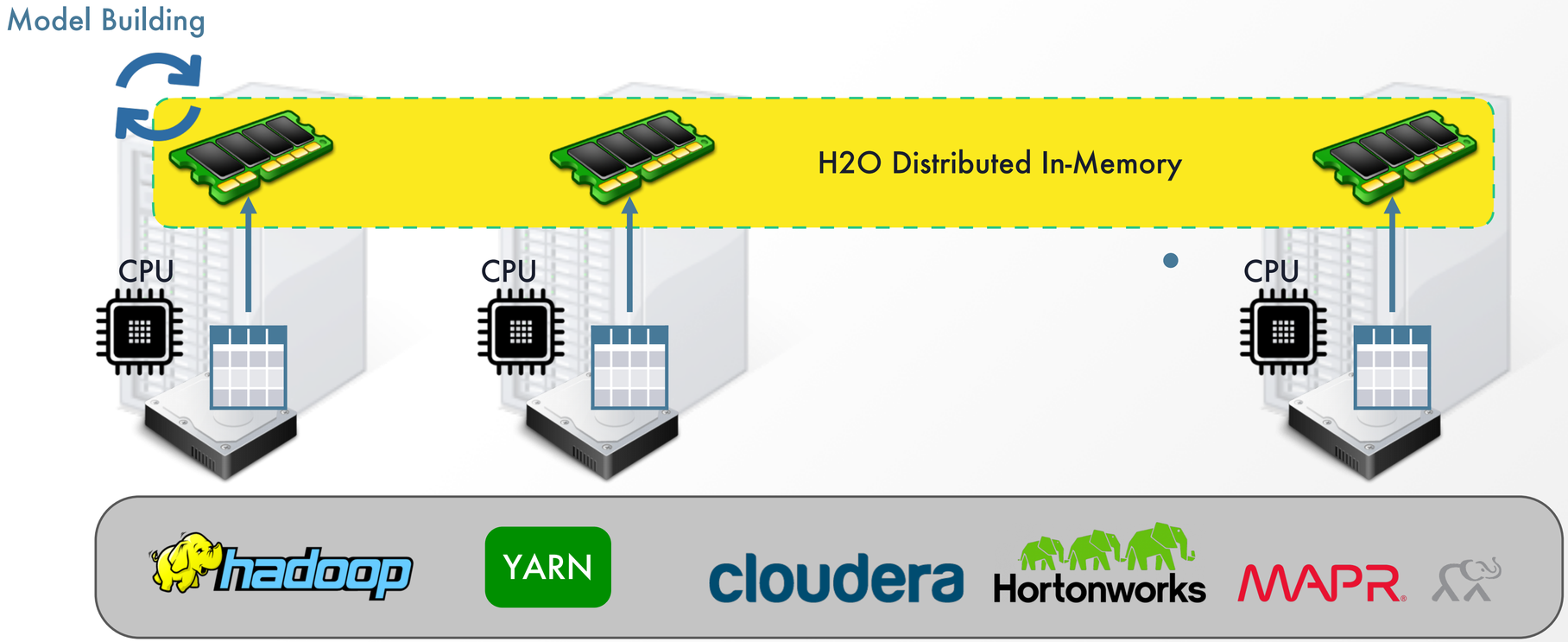
H2O Core

H2O Core

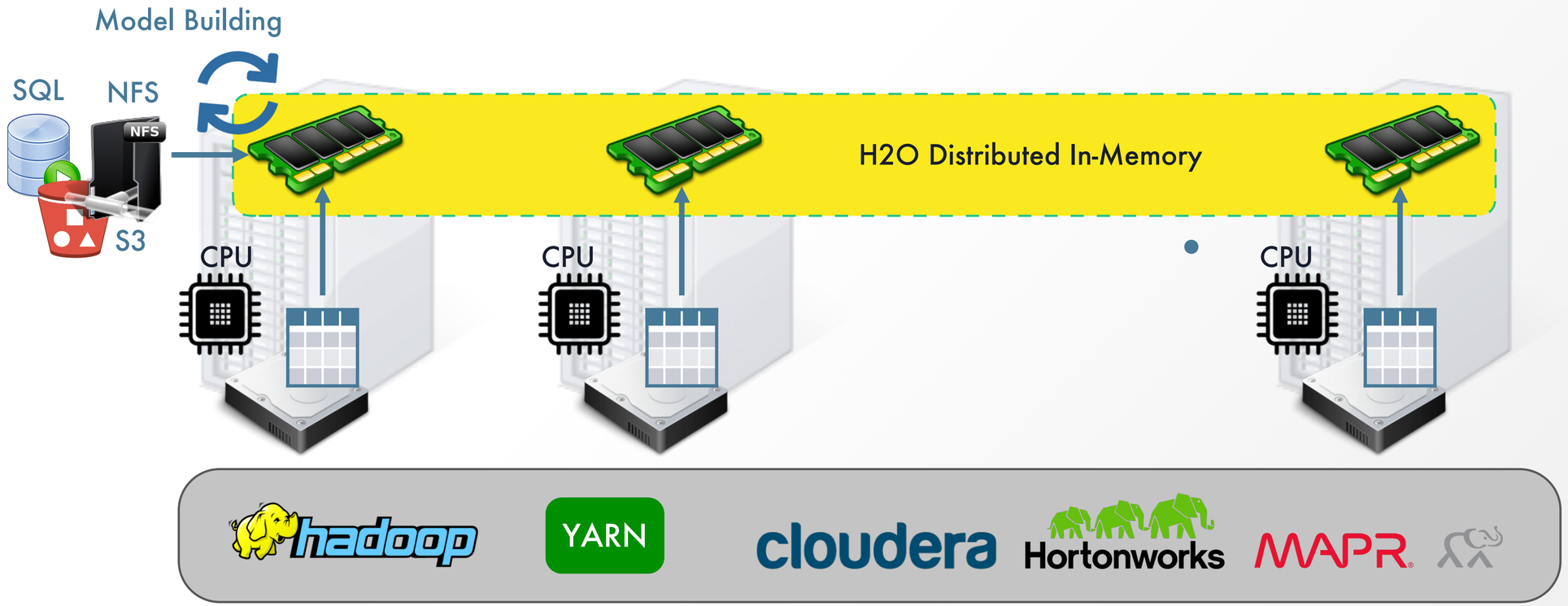
H2O Core



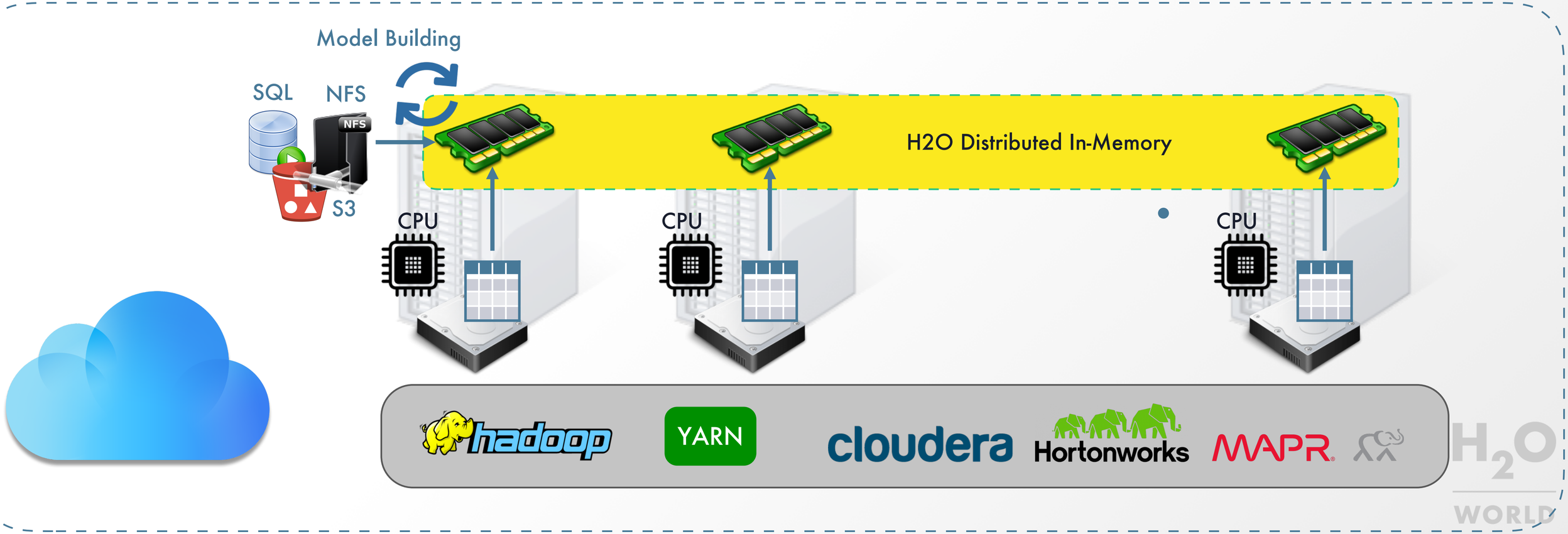
H2O Core with Hadoop



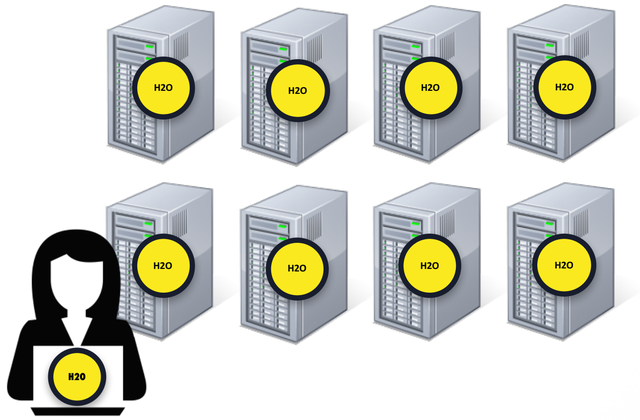
H2O Core with Other Data Sources



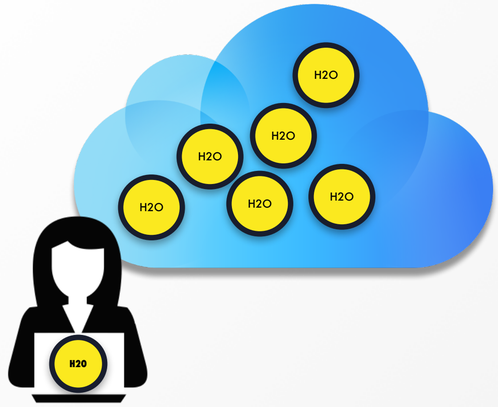
H2O Core on the Cloud



H2O Distributed Environments



distributed across multiple machines



distributed on the cloud

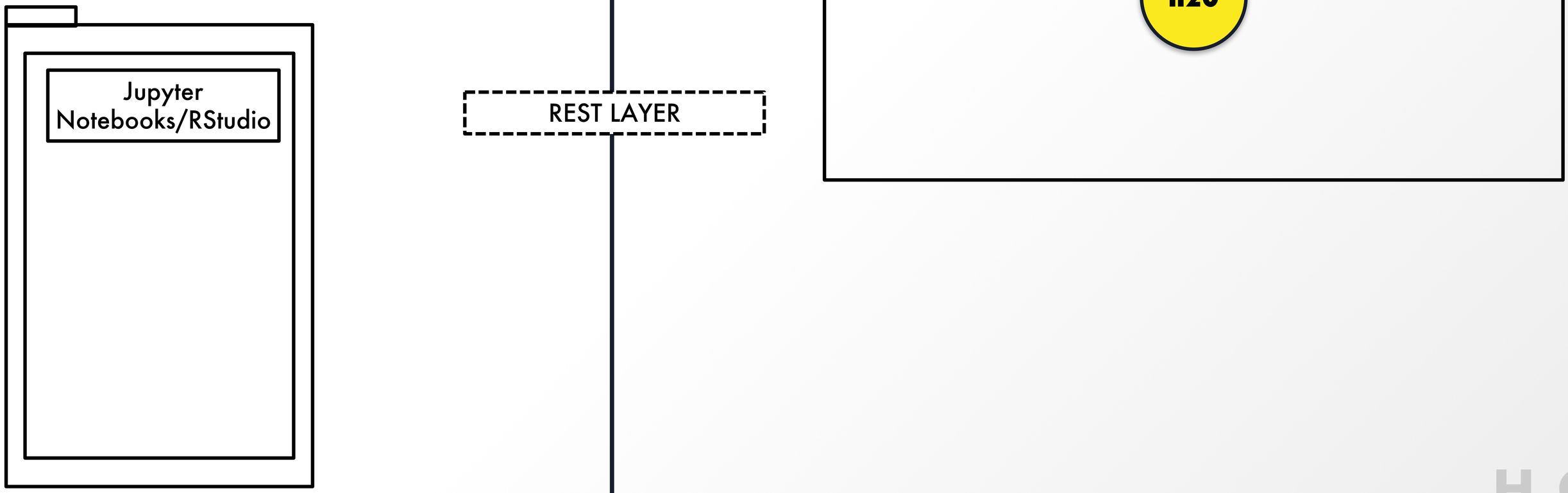
The H2O Python/R API

(how the client & cluster communicate)

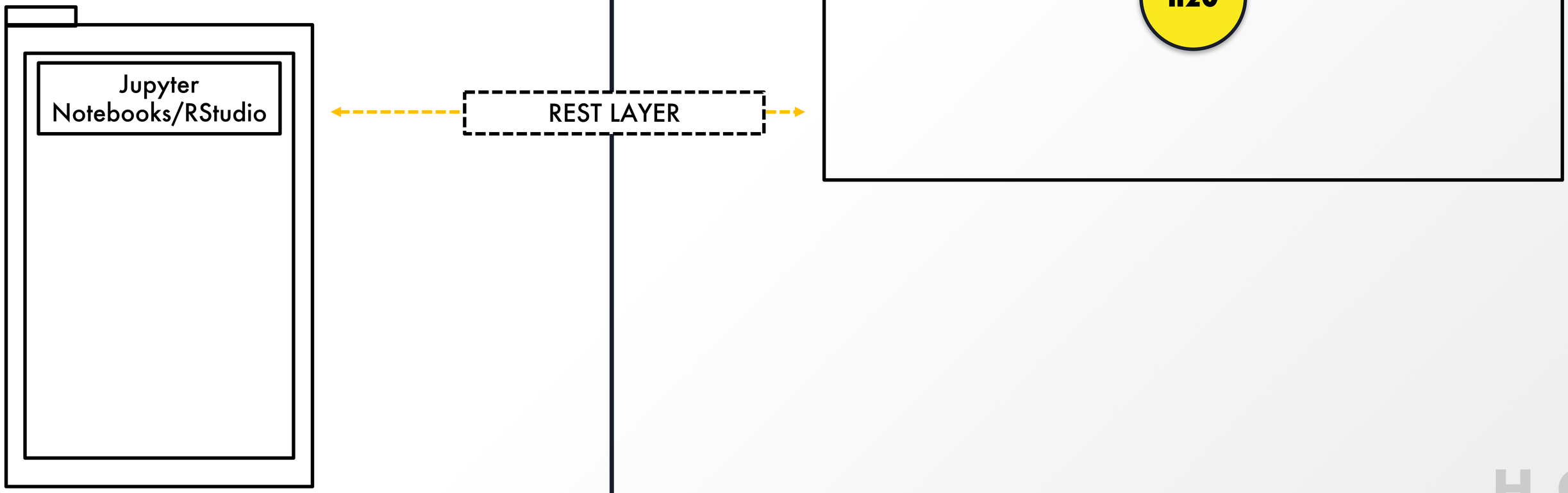
H2O Python/R API

H2O Python/R API

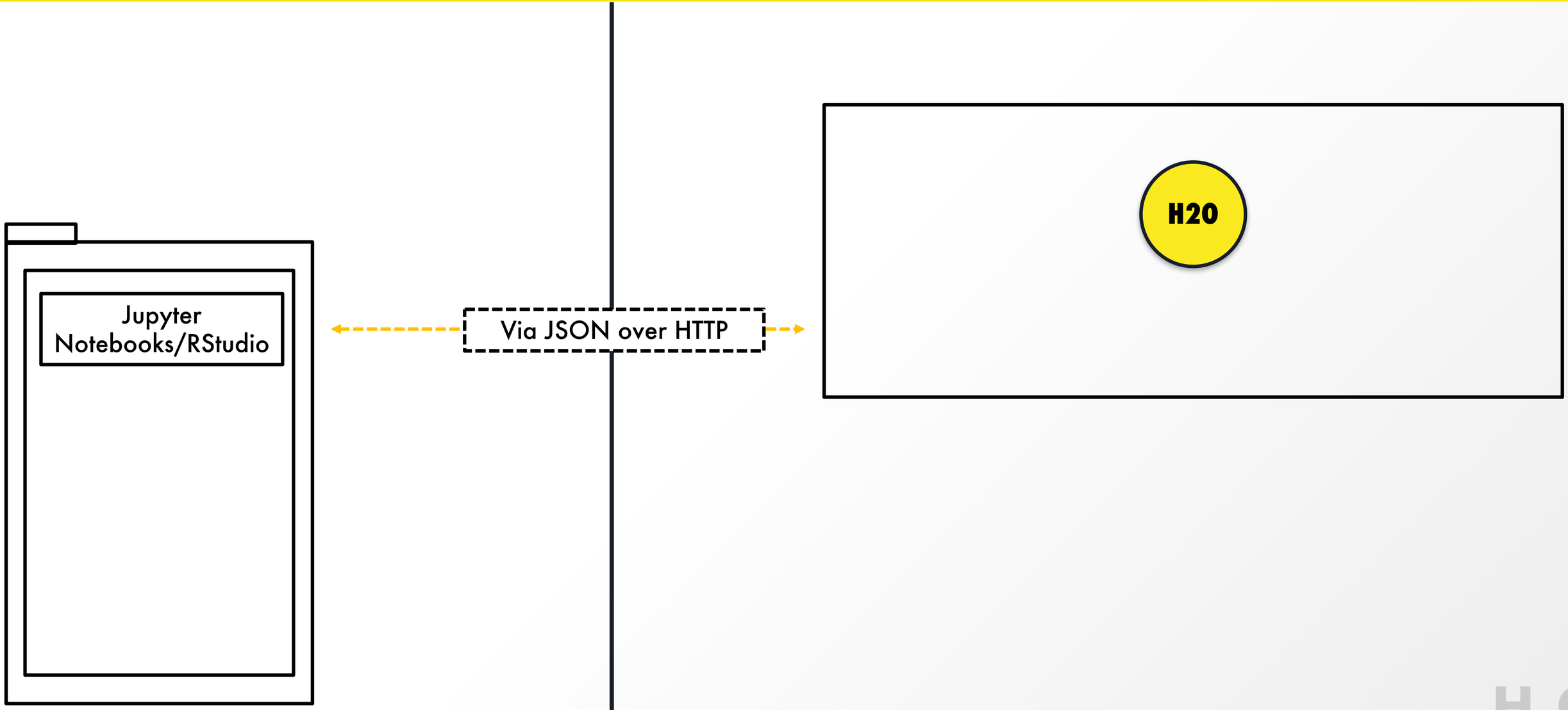
H2O Python/R API



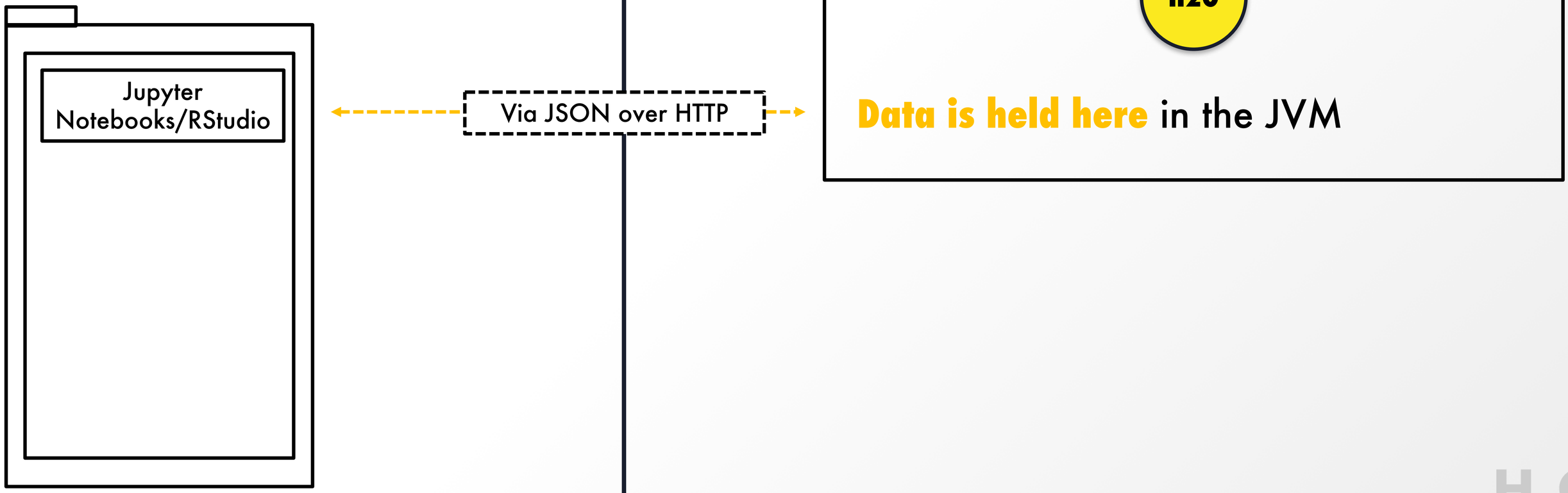
H2O Python/R API



H2O Python/R API

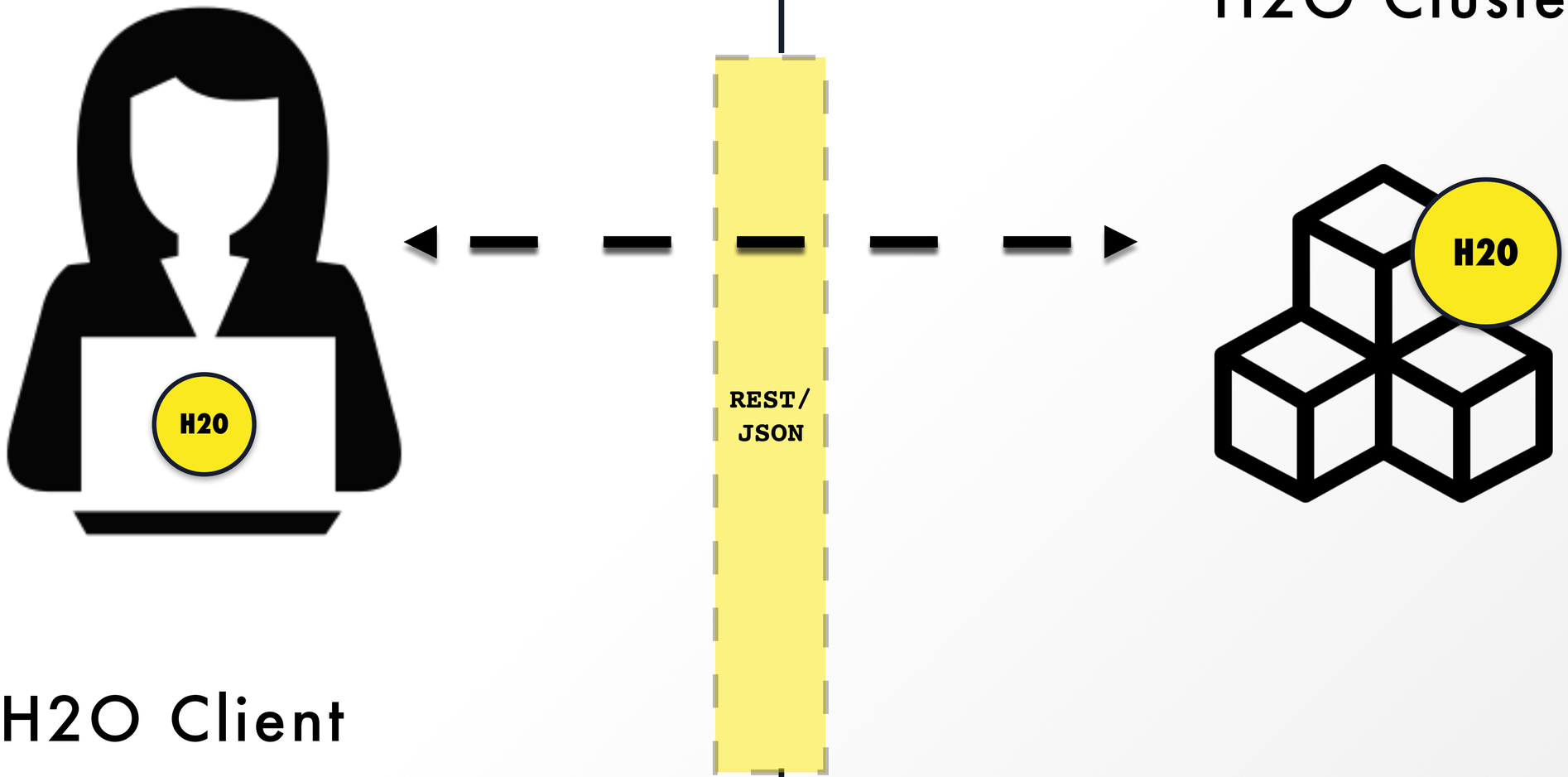


H2O Python/R API



Data is NOT in the python/R process

Client & Cluster Communication



Communication Layers: Interface

Standard Python Interface

the Client

Jupyter Notebook Interface

localhost:8888/notebooks/Untitled.ipynb?kernel_name=python3

jupyter Untitled Last Checkpoint: a few seconds ago (unsaved changes)

File Edit View Insert Cell Kernel Help

Code CellToolbar

```
In [1]: import h2o
        h2o.init()
```

```
Checking whether there is an H2O instance running at http
```

H2O cluster uptime:	54 secs
H2O cluster version:	3.16.0.2
H2O cluster version age:	21 days, 21 hours and 30 minutes
H2O cluster name:	H2O_from_python_laurend_53px3f
H2O cluster total nodes:	1
H2O cluster free memory:	3.541 Gb
H2O cluster total cores:	4

Terminal Interface

1. Shell

```
03:40:45 ~ python
Python 2.7.11 (default, Jan 22 2016, 08:29:18)
[GCC 4.2.1 Compatible Apple LLVM 7.0.2 (clang-700.1.81)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> import h2o
>>> h2o.init()
Checking whether there is an H2O instance running at http://localhost:54321.....
Attempting to start a local H2O server...
  Java Version: java version "1.8.0_73"; Java(TM) SE Runtime Environment (build 1
) 64-Bit Server VM (build 25.73-b02, mixed mode)
  Starting server from /usr/local/lib/python2.7/site-packages/h2o/backend/bin/h2o
  Ice root: /var/folders/k_/kpp1czqs3957vq2pr5qngck00000gn/T/tmpODqYLb
  JVM stdout: /var/folders/k_/kpp1czqs3957vq2pr5qngck00000gn/T/tmpODqYLb/h2o_laur
  JVM stderr: /var/folders/k_/kpp1czqs3957vq2pr5qngck00000gn/T/tmpODqYLb/h2o_laur
  Server is running at http://127.0.0.1:54321
Connecting to H2O server at http://127.0.0.1:54321... successful.
-------------------------  ----------------------------------------
H2O cluster uptime:         03 secs
H2O cluster version:        3.16.0.2
H2O cluster version age:    21 days, 21 hours and 29 minutes
H2O cluster name:           H2O_from_python_laurend_53px3f
H2O cluster total nodes:    1
H2O cluster free memory:    3.556 Gb
H2O cluster total cores:    4
H2O cluster allowed cores:  4
H2O cluster status:         accepting new members, healthy
H2O connection url:         http://127.0.0.1:54321
H2O connection proxy:
H2O internal security:      False
H2O API Extensions:         XGBoost, Algos, AutoML, Core V3, Core V4
Python version:             2.7.11 final
-------------------------  ----------------------------------------
>>>
```

H2O.ai

Communication Layers: Code Script

Python Notebook

the Client

Python Notebook using H2O Package

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

In [ ]:

```
import h2o
from h2o.estimators.glm import H2OGeneralizedLinearEstimator
h2o.init()

# import the boston dataset:
# this dataset looks at features of the boston suburbs and predicts median housing prices
# the original dataset can be found at https://archive.ics.uci.edu/ml/datasets/Housing
boston = h2o.import_file("https://s3.amazonaws.com/h2o-public-test-data/smalldata/gbm_test/Bosto

# set the predictor names and the response column name
predictors = boston.columns[:-1]
# set the response column to "medv", the median value of owner-occupied homes in $1000's
response = "medv"

# convert the chas column to a factor (chas = Charles River dummy variable (= 1 if tract bounds
boston['chas'] = boston['chas'].asfactor()

# split into train and validation sets
train, valid = boston.split_frame(ratios = [.8])


# try using the `alpha` parameter:
# initialize the estimator then train the model
boston_glm = H2OGeneralizedLinearEstimator(alpha = .25)
boston_glm.train(x = predictors, y = response, training_frame = train, validation_frame = valid)

# print the mse for the validation data
print(boston_glm.mse(valid=True))
```

H2O.ai

Communication Layers: A Command

Python Commands

the Client

Importing Big Data with Python Code

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

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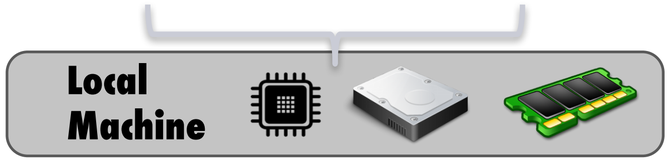
```

h2o.import_file(…)



H2O.ai

Communication Layers: A Command

Python Commands

the Client

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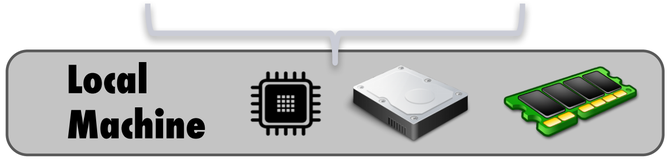

Path to Your Dataset

`h2o.import_file(…)`

Fourth: Communicate

`h2o.import_file(…)`
`requests file import`

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

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REST / JSON

H2O Cluster

Local Machine

H2O WORLD

Fifth: Cluster Does Heavy Lifting

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

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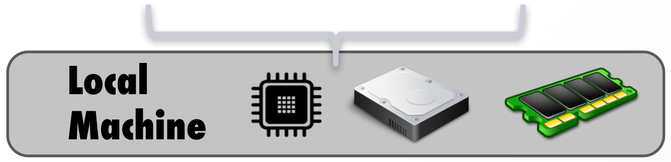


H2O Cluster

REST/
JSON

H2O WORLD

Fifth: Cluster Does Heavy Lifting

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

In [ ]:

```
import h2o
from h2o.estimators.glm import H2OGeneralizedLinearEstimator
h2o.init()

# import the boston dataset:
# this dataset looks at features of the boston suburbs and predicts median housing prices
# the original dataset can be found at https://archive.ics.uci.edu/ml/datasets/Housing
boston = h2o.import_file("https://s3.amazonaws.com/h2o-public-test-data/smalldata/gbm_test/Bostc

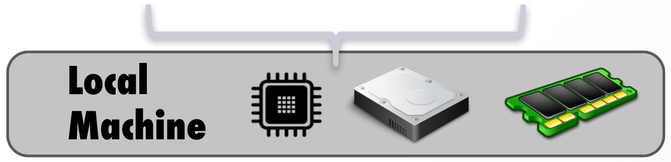
# set the predictor names and the response column name
predictors = boston.columns[:-1]
# set the response column to "medv", the median value of owner-occupied homes in $1000's
response = "medv"

# convert the chas column to a factor (chas = Charles River dummy variable (= 1 if tract bounds
boston['chas'] = boston['chas'].asfactor()

# split into train and validation sets
train, valid = boston.split_frame(ratios = [.8])


# try using the `alpha` parameter:
# initialize the estimator then train the model
boston_glm = H2OGeneralizedLinearEstimator(alpha = .25)
boston_glm.train(x = predictors, y = response, training_frame = train, validation_frame = valid)

# print the mse for the validation data
print(boston_glm.mse(valid=True))
```



REST/
JSON

H2O Cluster

H2O WORLD

Fifth: Cluster Does Heavy Lifting

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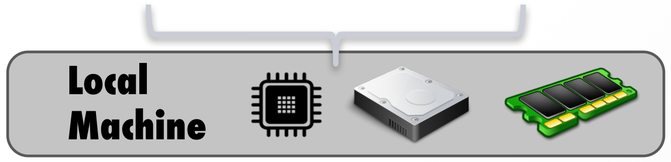
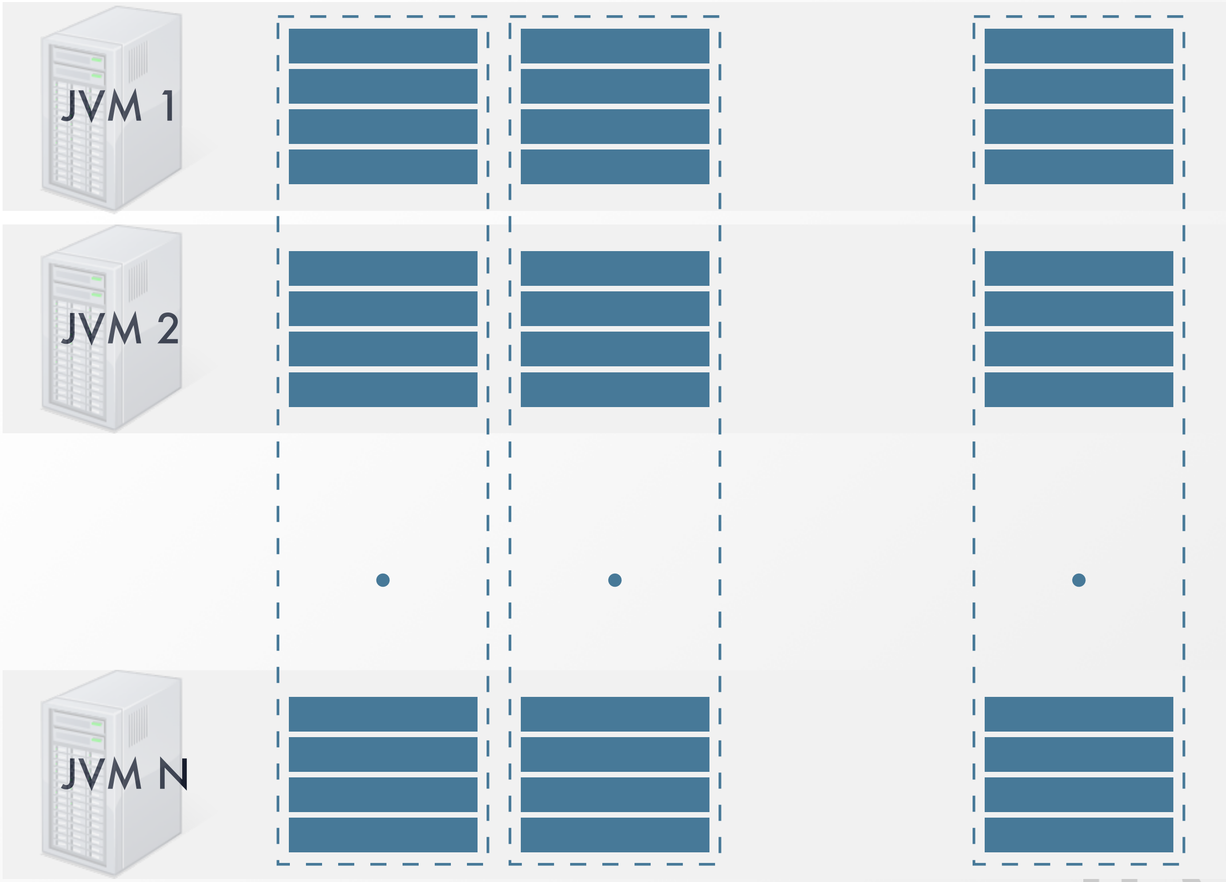


REST/
JSON

H2O Cluster



H2O WORLD

Fifth: Cluster Does Heavy Lifting

File Edit View Insert Cell Kernel Help | Python 3

Code | CellToolbar

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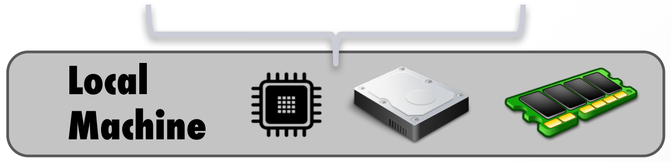

REST/
JSON

H2O Cluster

x_1	x_2	x_3	...	x_p	y

H2O WORLD

H2O Client

cluster returns frame key

File Edit View Insert Cell Kernel Help Python 3

Code CellToolbar

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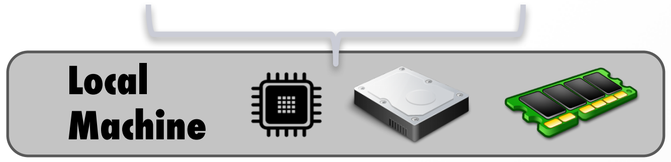


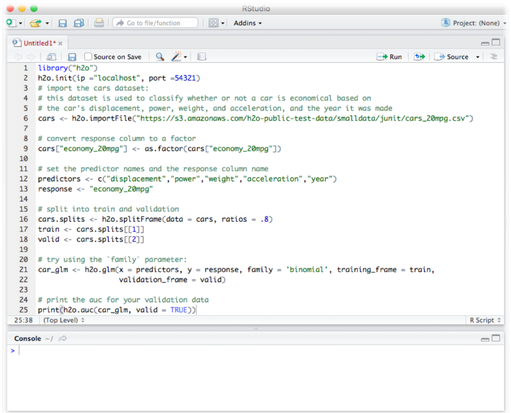
REST/ JSON

x_1	x_2	x_3	...	x_p	y

H2O WORLD

What does the Client Do?

Clients Only Tells the Cluster What to Do

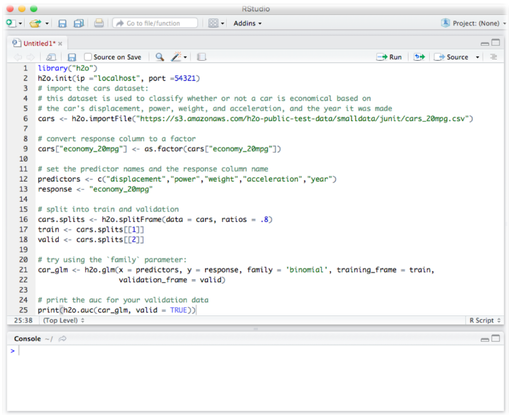


Hi Cluster,
Can you please get me …

H2O.ai

Client Only Passes Requests

Big Data Never Flows Through The Client
Unless **Explicitly** Asked



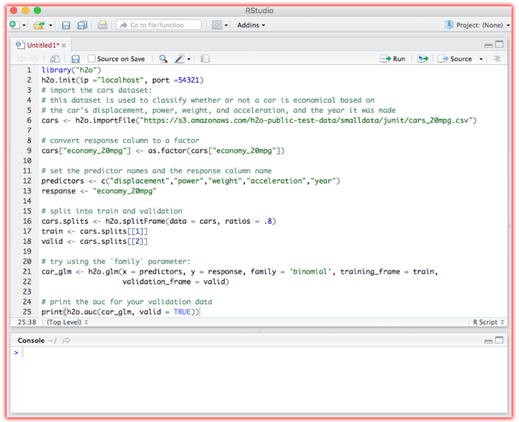
No, you take care of the heavy lifting

H2O.ai

What if?

Pulling Big Data into Python/R Can Overwhelm Your Session

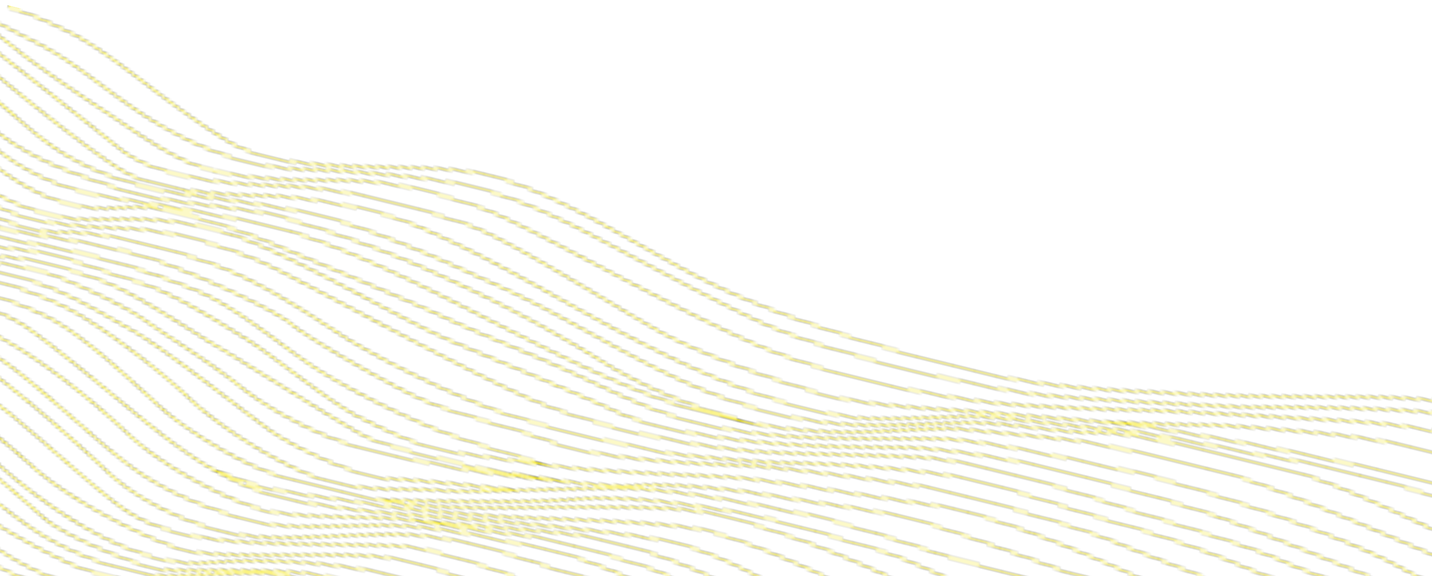
```
my_big_dataframe.as_data_frame()
```



H2O.ai

Automatic Machine Learning (AutoML)

Scalable Automatic Machine Learning



AutoML Agenda

- **The Machine Learning Pipeline**
- What is Automatic Machine Learning?
- How to Use H2O's AutoML

AutoML Agenda

- The Machine Learning Pipeline
- What is Automatic Machine Learning? **(Feature Preprocessing)**
- How to Use H2O's AutoML

AutoML Agenda

- The Machine Learning Pipeline
- What is Automatic Machine Learning?**(Feature Engineering)**
- How to Use H2O's AutoML

AutoML Agenda

- The Machine Learning Pipeline
- What is Automatic Machine Learning?**(Hyperparameter Search)**
- How to Use H2O's AutoML

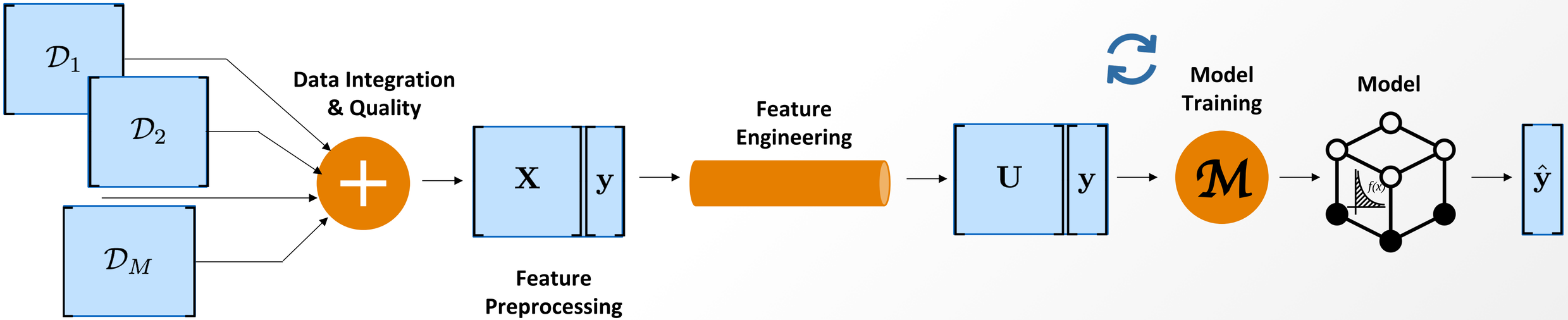
AutoML Agenda

- The Machine Learning Pipeline
- What is Automatic Machine Learning?**(Stacked Ensembles)**
- How to Use H2O's AutoML

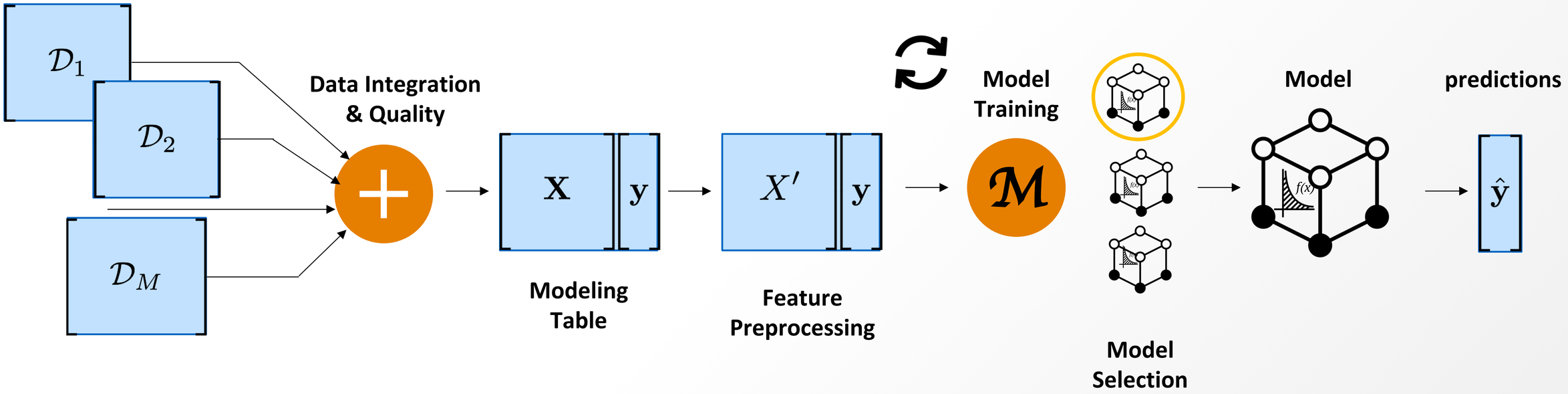
AutoML Agenda

- The Machine Learning Pipeline
- What is Automatic Machine Learning?
- **How to Use H2O's AutoML** (**more hands-on!**)

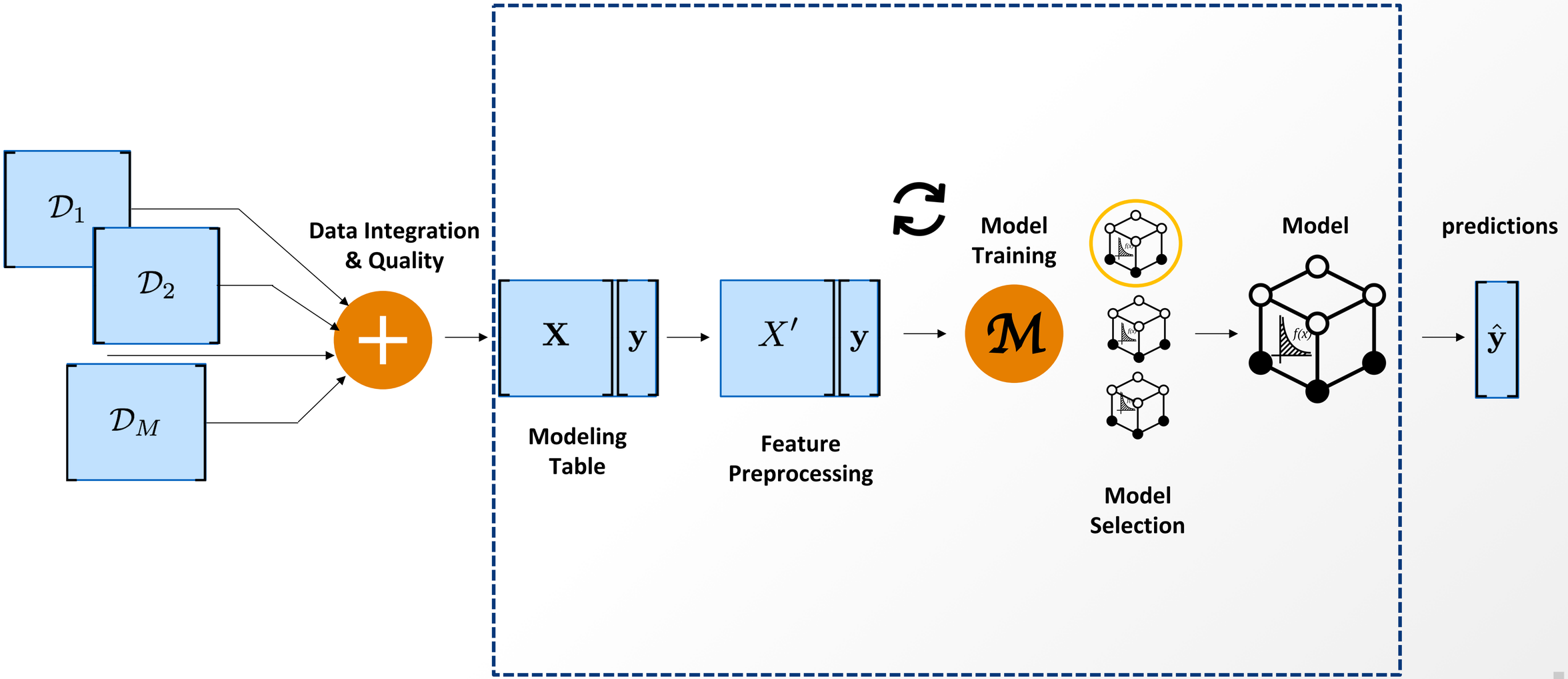
The Machine Learning Pipeline



Updated Machine Learning Pipeline



Where Automatic Machine Learning Fits



Automatic ML Overview

- **Feature Preprocessing**
- **Feature Engineering**
- Hyperparameter Search
- Ensembles

Automatic ML Overview

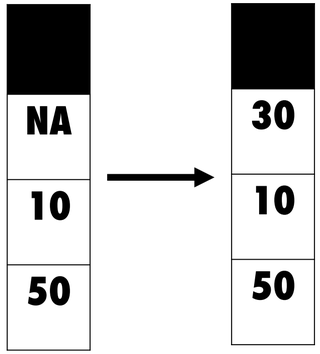
- **Feature Preprocessing**
- **Feature Engineering**

} Distinction Sometimes Fuzzy

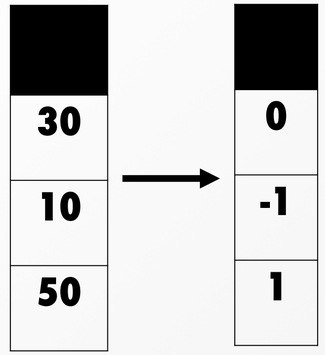
- Hyperparameter Search
- Ensembles

Feature Preprocessing

Missing Values

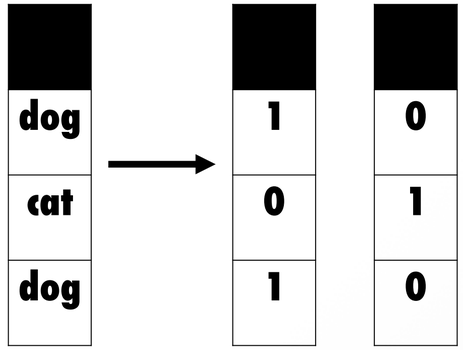


Standardization

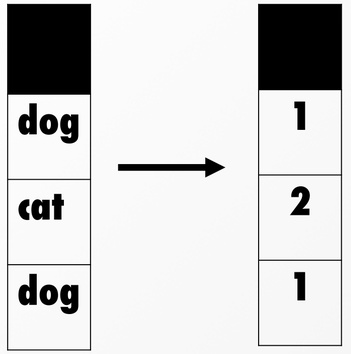


Feature Preprocessing

Handling Categorical Columns

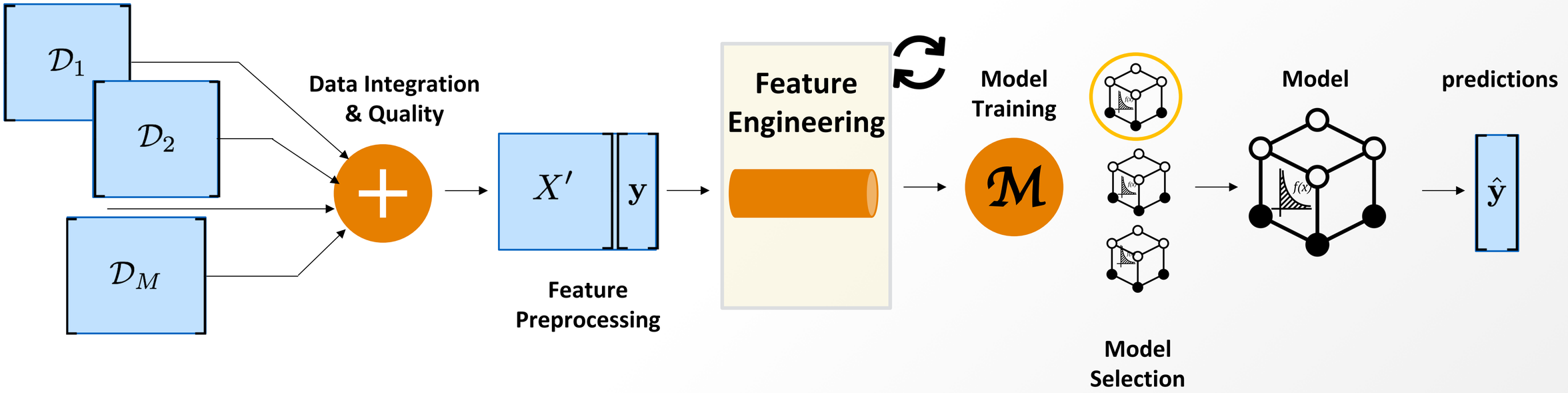


One-hot Encoding



Label Encoder

Adding in Feature Engineering



Feature Engineering

Domain Expertise

Timestamp
jan/02/2017
march/03/2019
dec/11/2018

→

Month	Day	Year
01	02	2017
03	03	2019
12	11	2018

Date Expansion

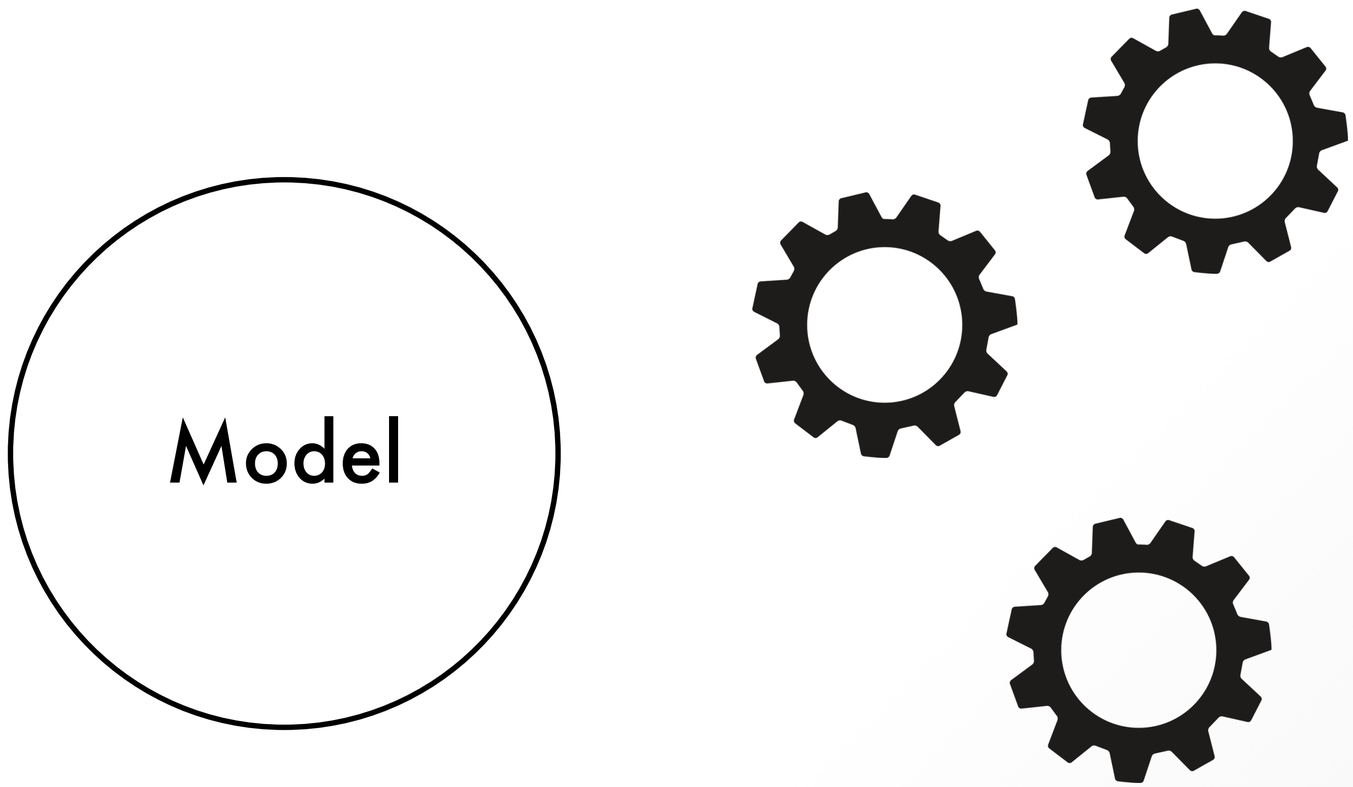
Automatic ML Overview

- ~~Feature Preprocessing~~
- ~~Feature Engineering~~
- **Hyperparameter Search** (**part of H2O AutoML**)
- Ensembles

What are Hyperparameters?

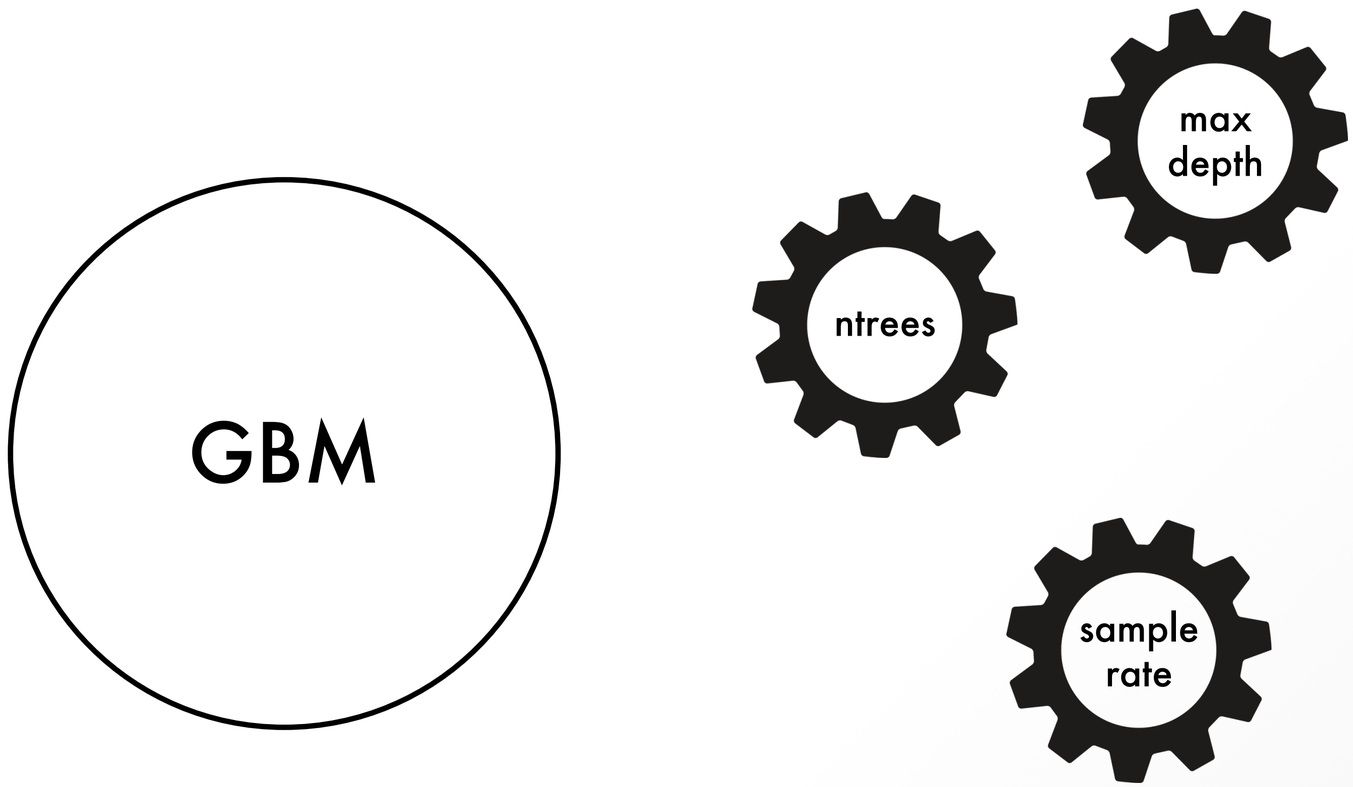
(a quick review)

What are Model Hyperparameters?



Every model comes with knobs

What are Model Hyperparameters?



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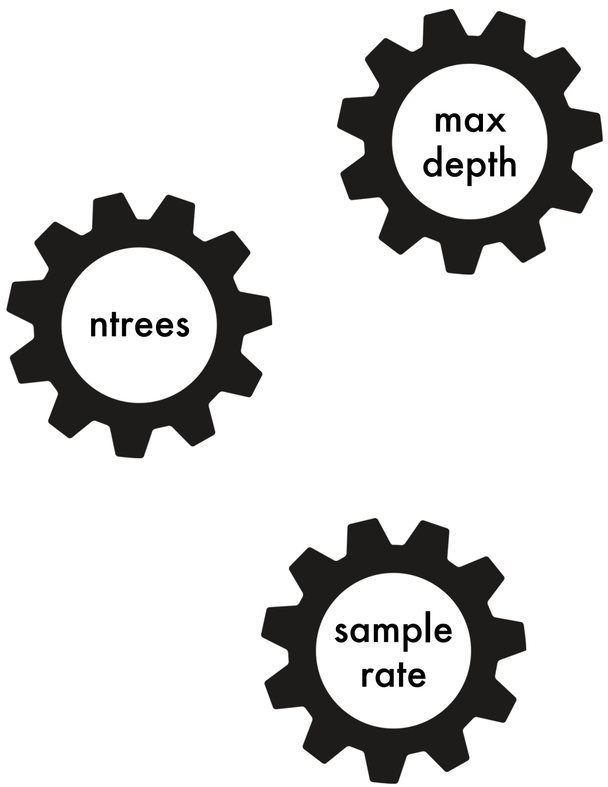
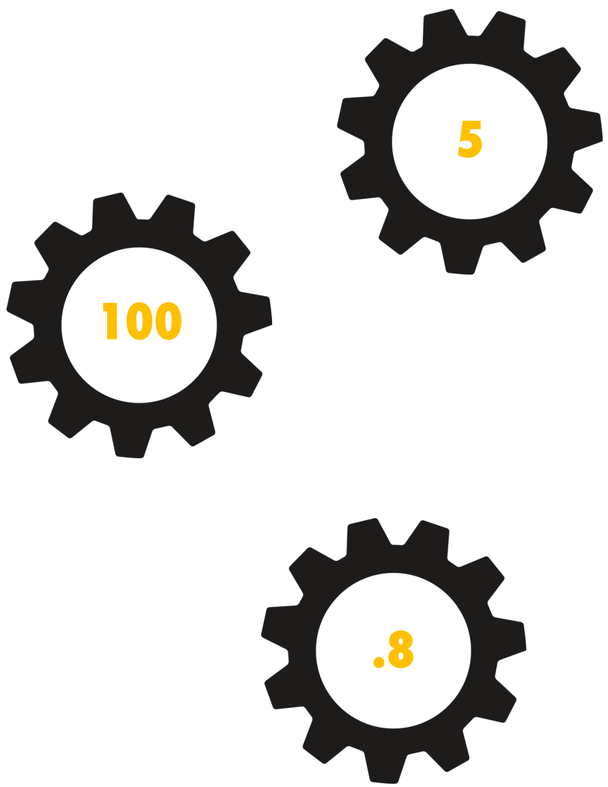
What are Hyperparameter?



Unlike regular model parameters, hyperparameters are not learned from the data

The user has to set the hyperparameters values

What are Hyperparameter?



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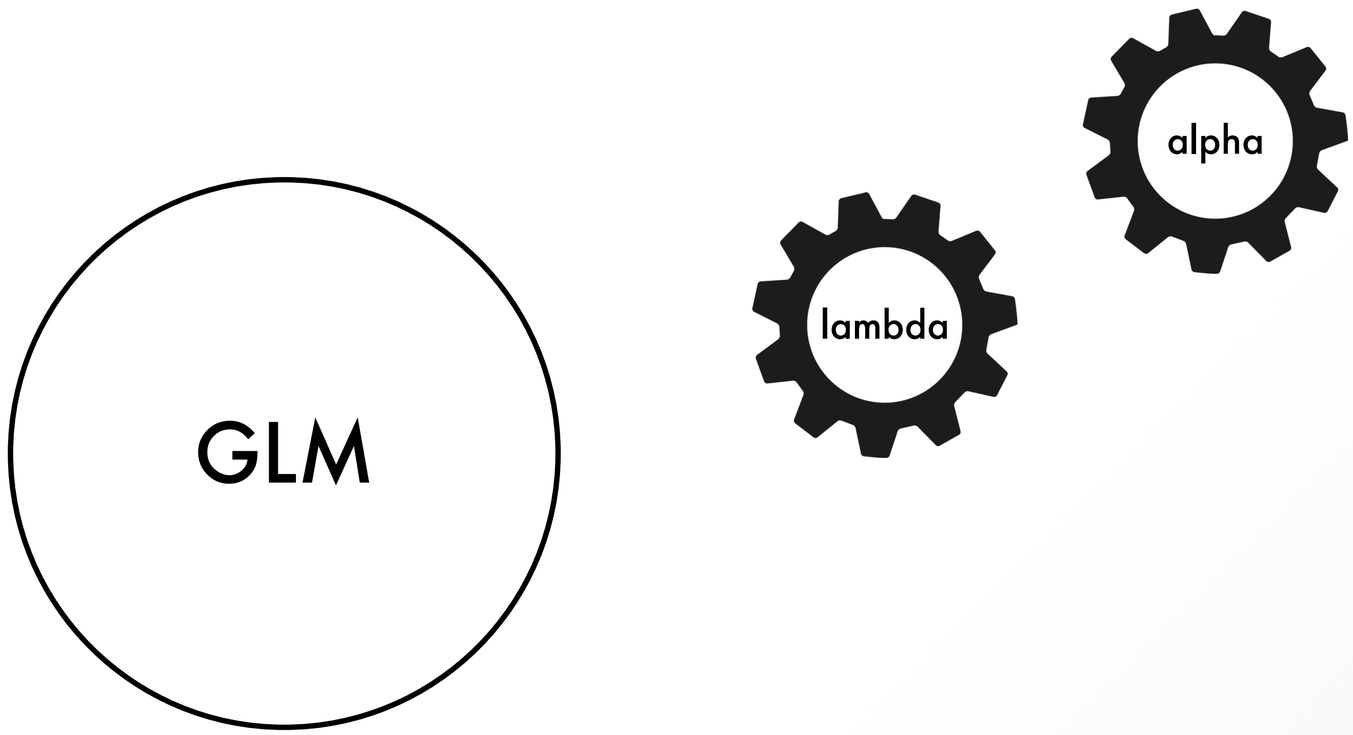
What are GLM's Hyperparameters?



GLM Model Parameters

$$\max_{\beta,\beta_0} \sum_{i=1}^{N} \log f\left(y_i;\beta,\beta_0\right) - \lambda\left(\alpha\|\beta\|_1 + \frac{1}{2}(1-\alpha)\|\beta\|_2^2\right)$$

GLM Model Parameters

$$\max_{\beta,\beta_0} \sum_{i=1}^{N} \log f\left(y_i; \beta, \beta_0\right) - \lambda \left(\alpha \|\beta\|_1 + \frac{1}{2}(1-\alpha)\|\beta\|_2^2 \right)$$

GLM Hyperparameter

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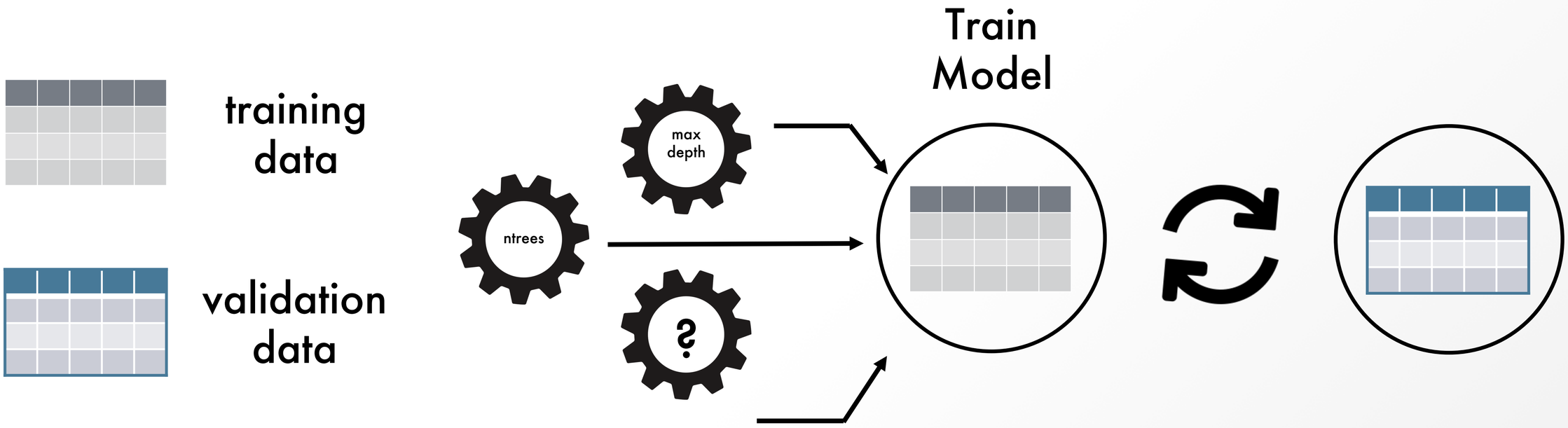
Model Building: Hyperparameter Search

4 Main Ways:

- Manual Model Tuning
- Cartesian Grid Search
- Random Grid Search*
- Bayesian Hyperparameter Optimization

*What AutoML Uses

Manual Model Tuning



Split Dataset

Specify Hyperparameter Values

Validate Performance

Manual Model Tuning

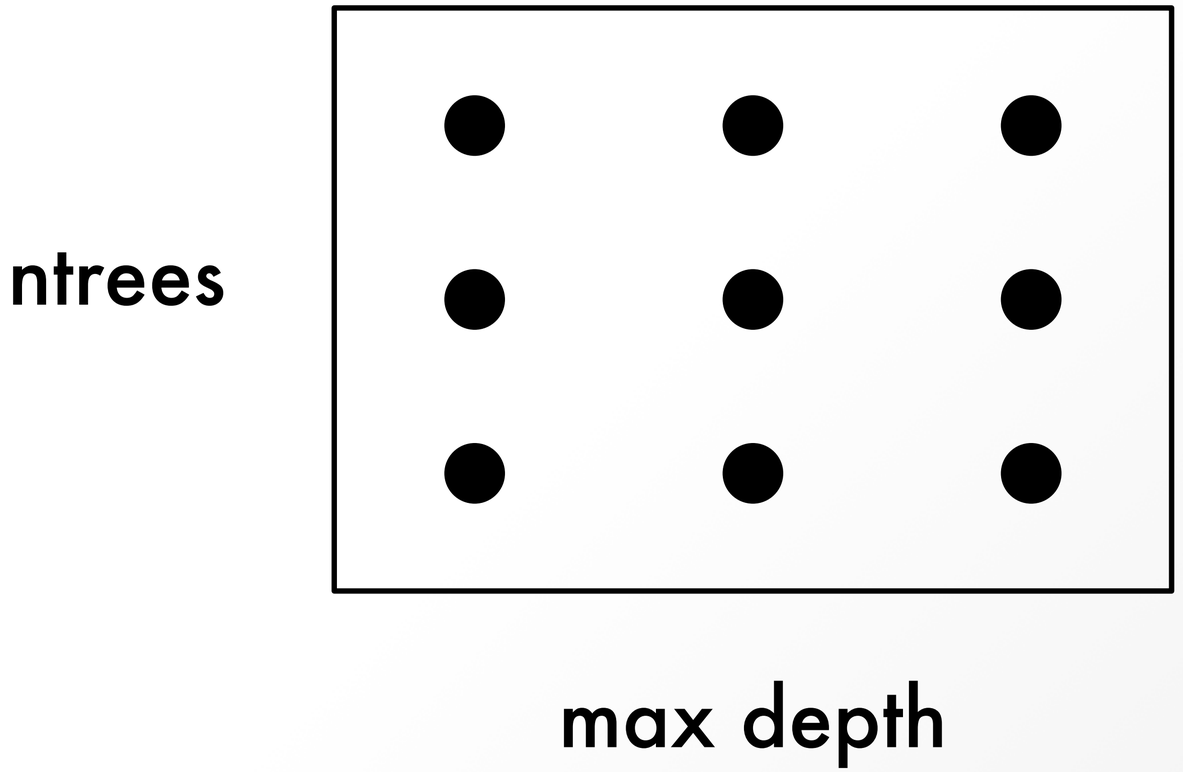
How did you do?

- Not so good: **Repeat** Process
- GOOD! : Stop

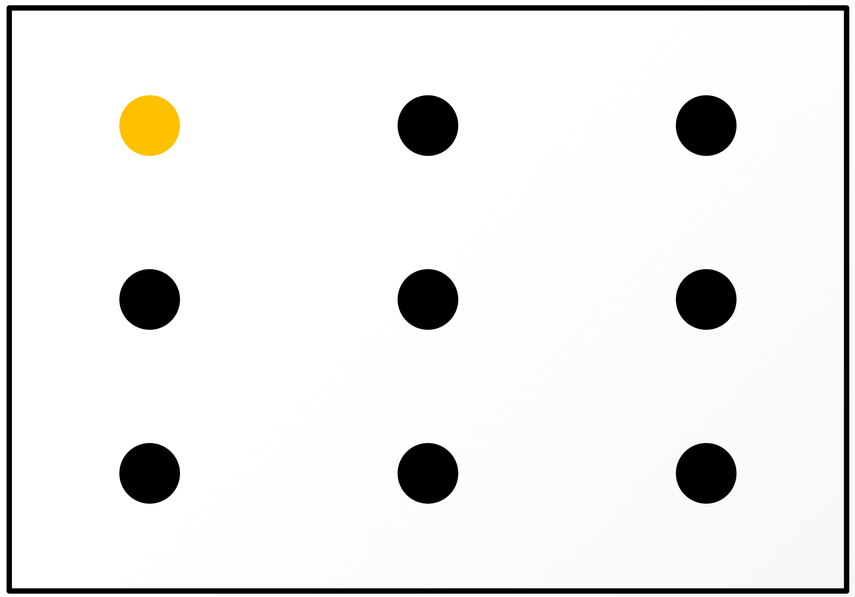
Cartesian Grid Search

AKA Exhaustive Search: Tries **Every Combination**

Cartesian Grid Search



Cartesian Grid Search

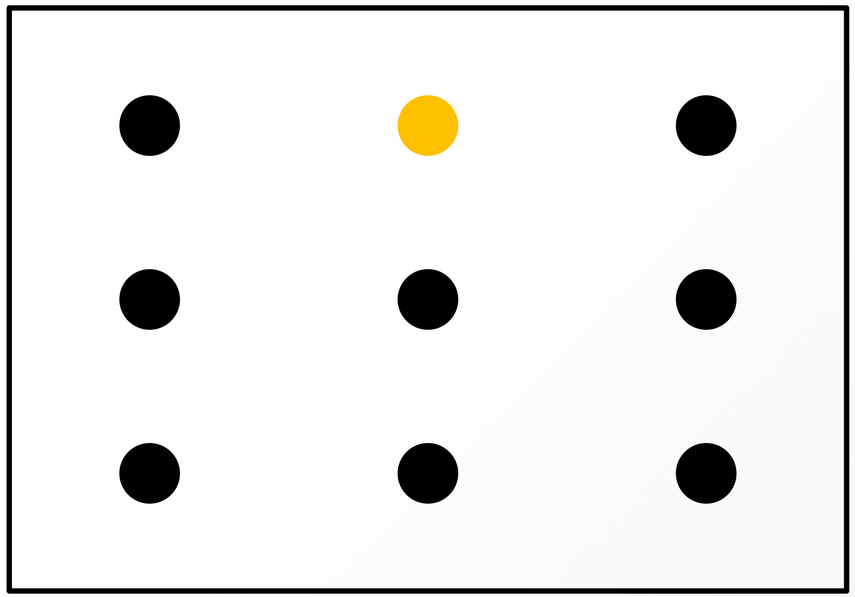


single trial

ntrees = 1000

max depth = 5

Cartesian Search

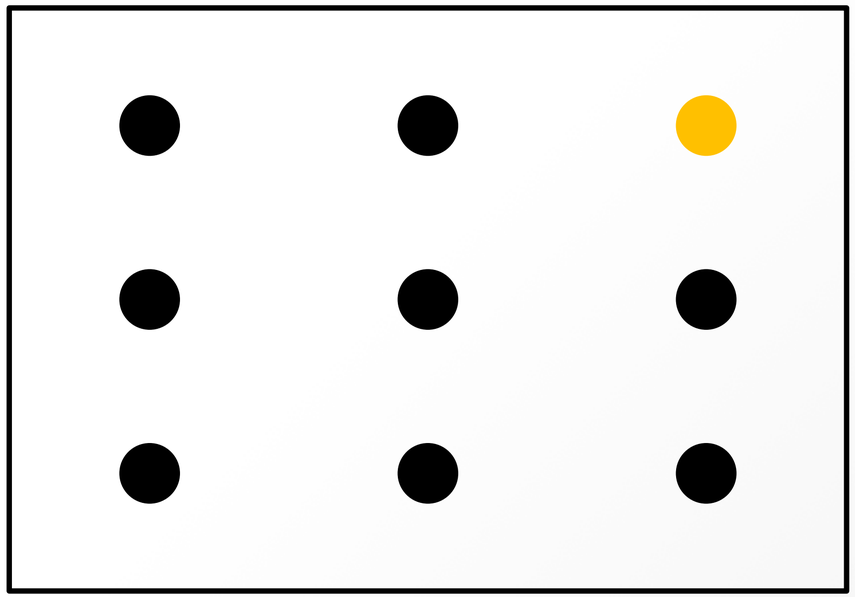


single trial

ntrees = 1000

max depth = 10

Cartesian Search

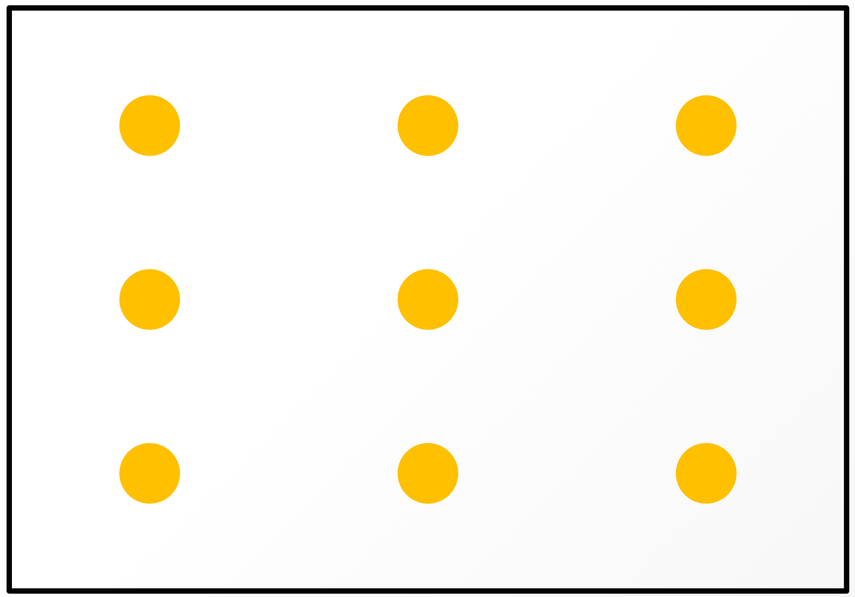


single trial

ntrees = 1000

max depth = 15

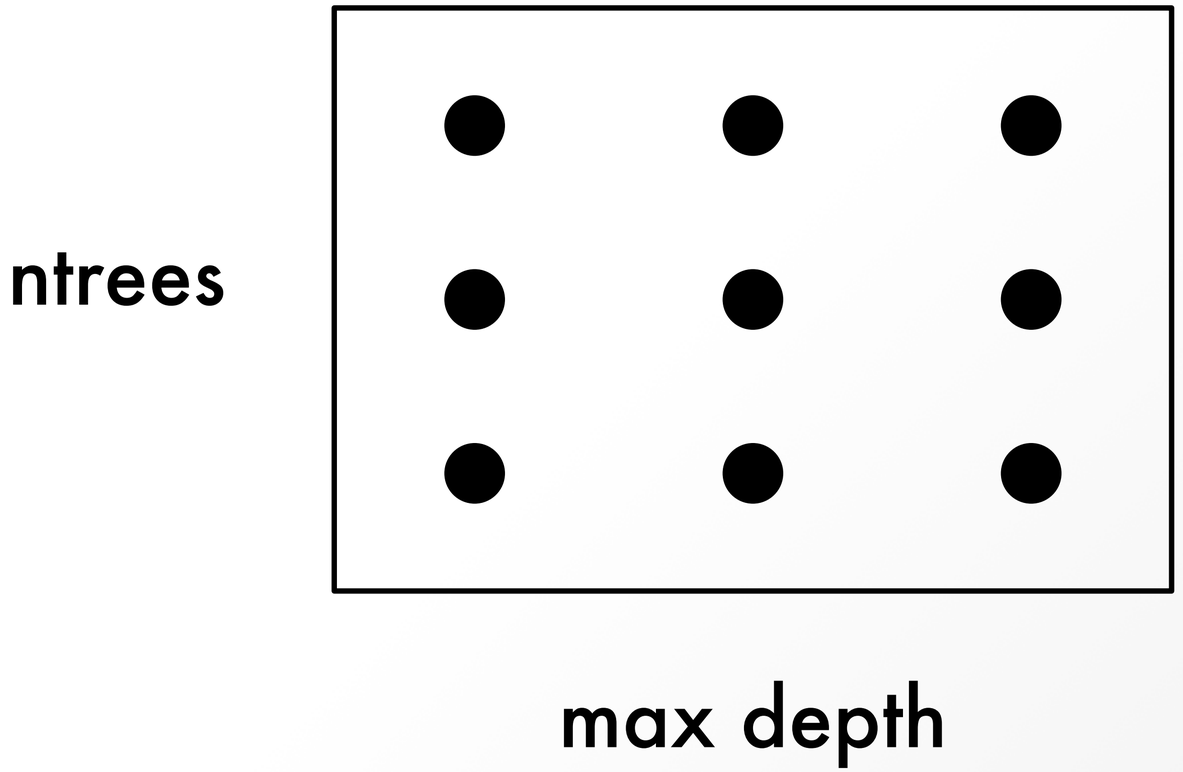
Cartesian Grid Search



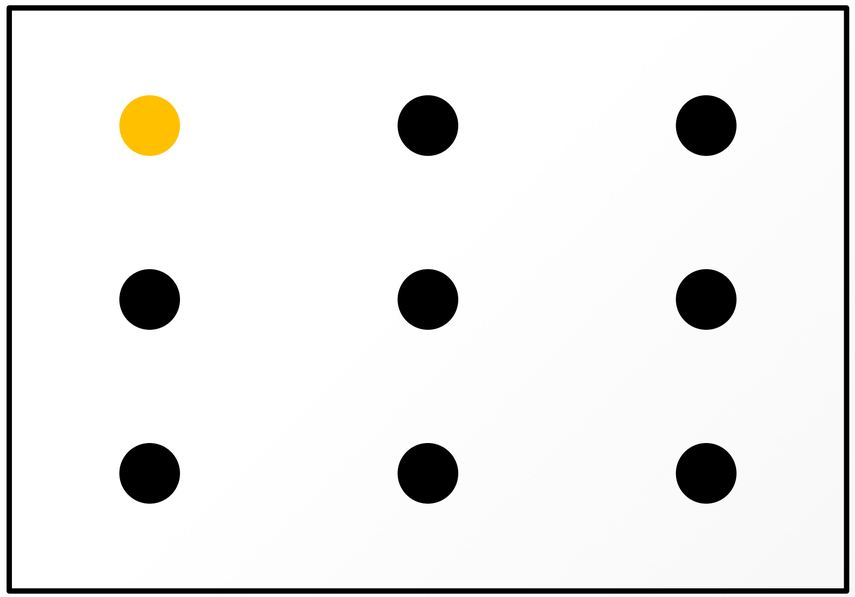
Cartesian Grid Search

Complete Exploration

Random Grid Search



Random Grid Search

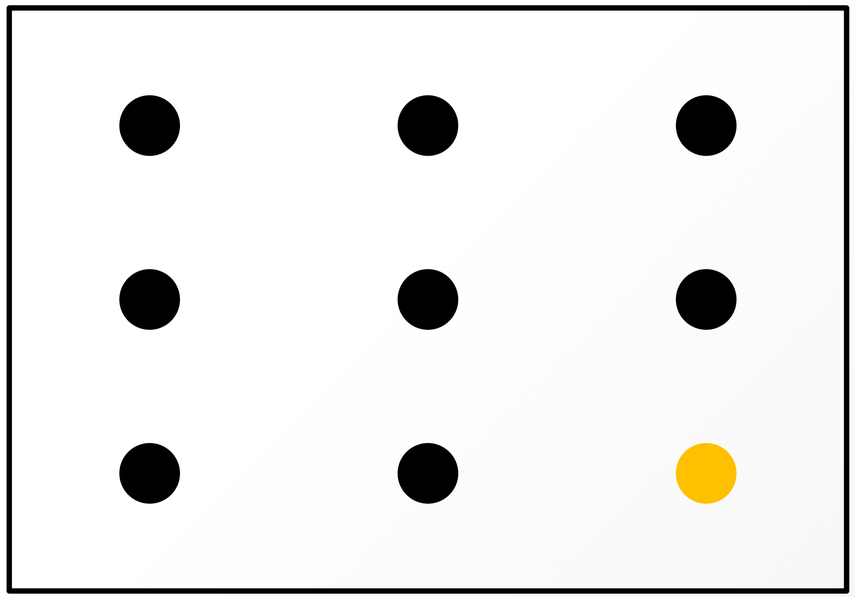


single trial

ntrees = 1000

max depth = 5

Random Grid Search

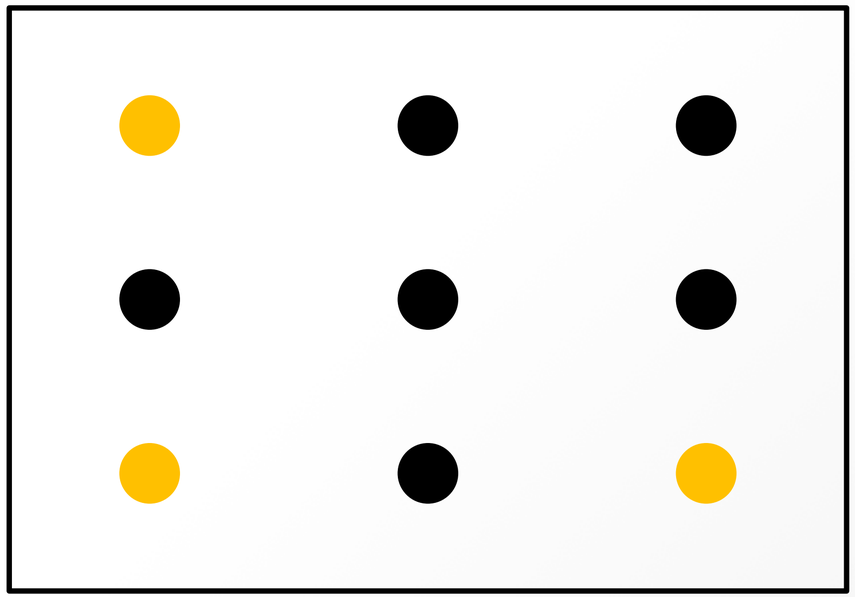


single trial

ntrees = 3000

max depth = 15

Random Grid Search

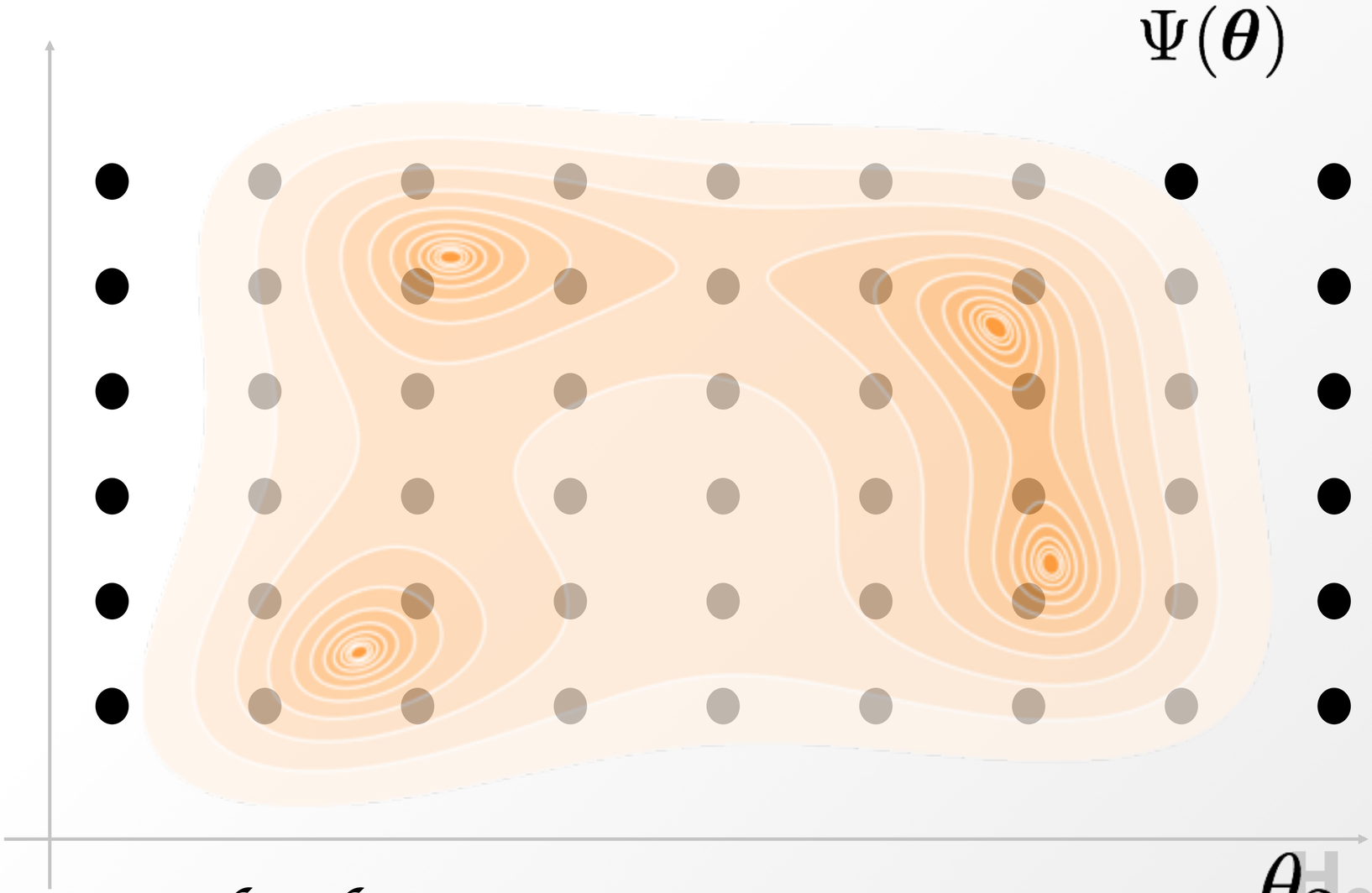


Random Grid Search

explores more in less time

Other ways to Optimize?

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta} \in \boldsymbol{\Theta}} \Psi(\boldsymbol{\theta})$$



$$\boldsymbol{\theta} = (\theta_1, \theta_2) = (ntrees, max\_depth)$$

Bayesian Optimization: An Analogy

Consider the following question:

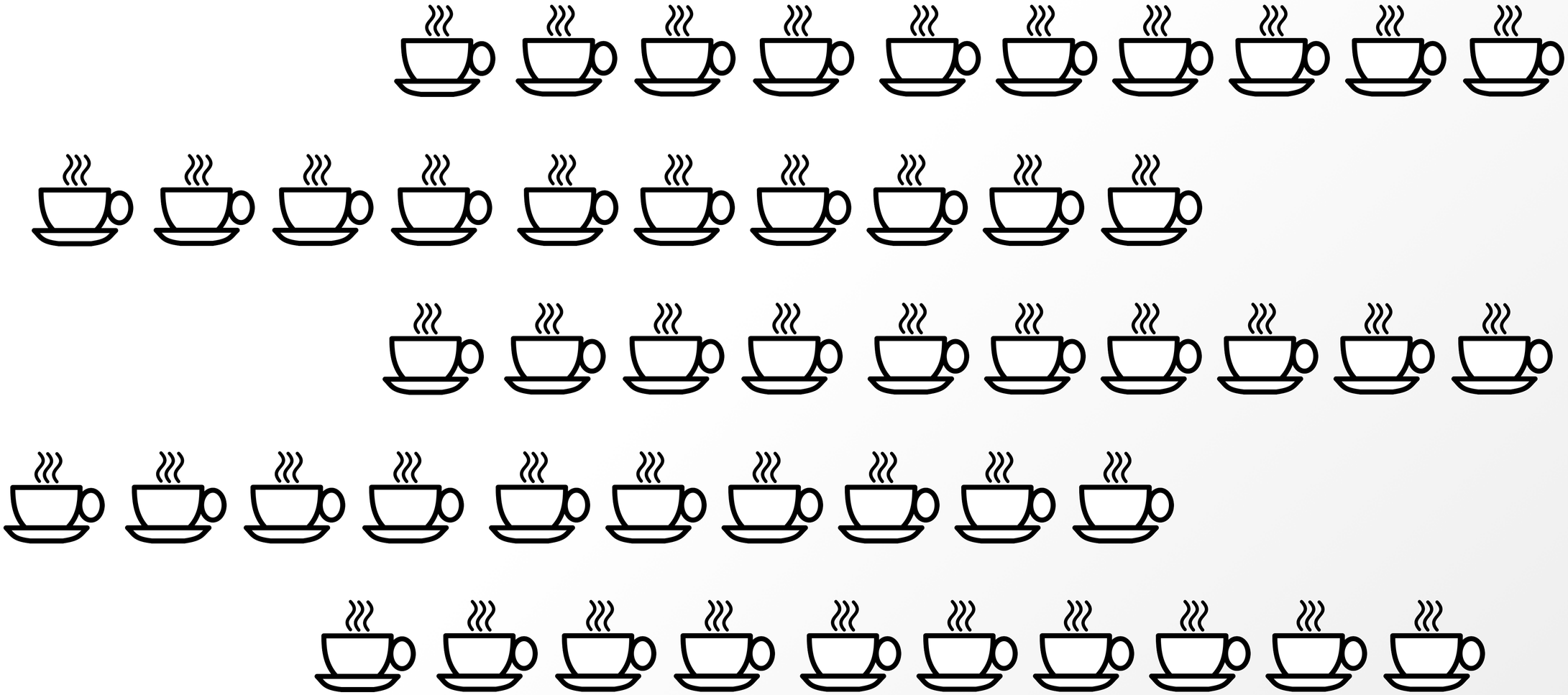
How would you make the **best cup** of coffee in world?

Given:

1. You have access to **every coffee** bean in the world
2. You have **every coffee instrument** ever invented
3. You only have **ONE WEEK**

Bayesian Optimization: An Analogy

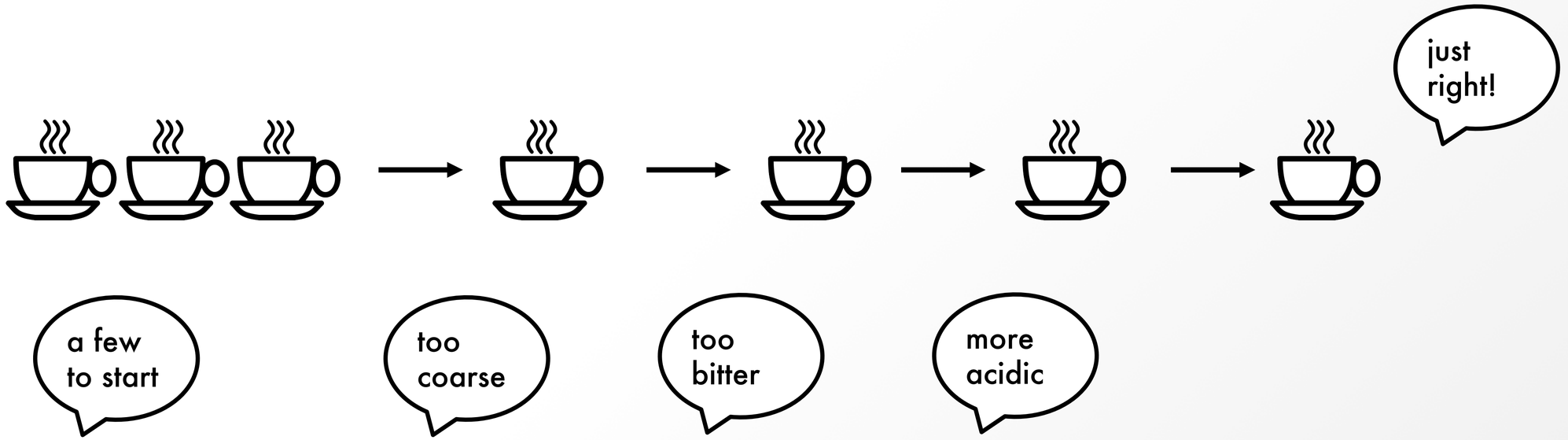
you could brew all the coffee!



Bayesian Optimization: An Analogy

What if you had a way to know how to **adjust the settings**

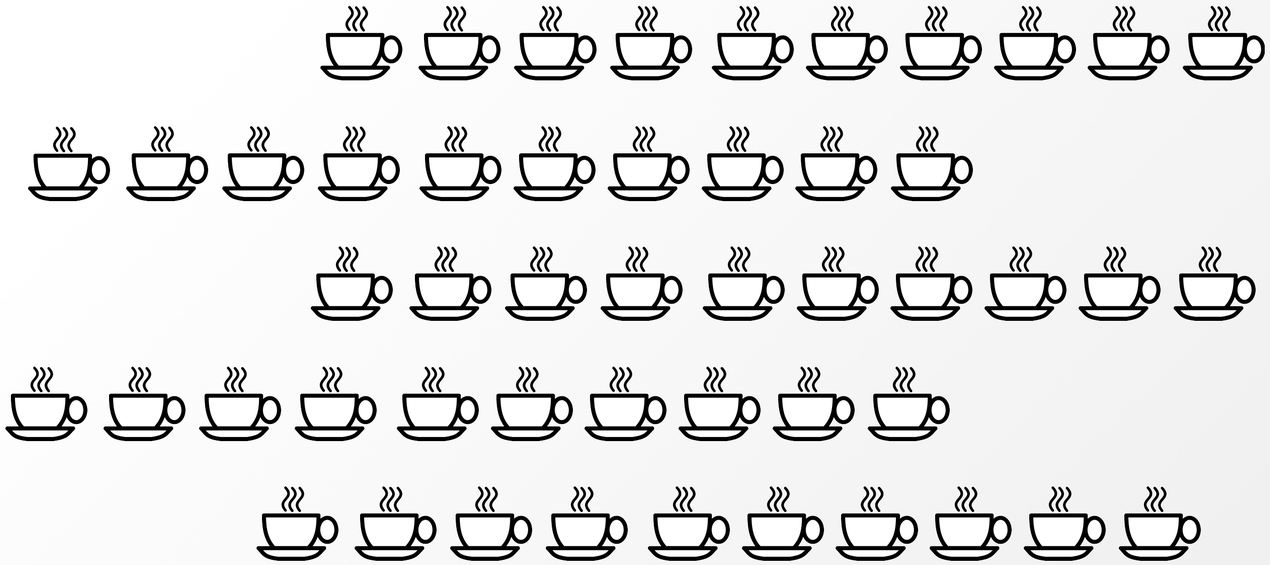
after every cup of coffee



Bayesian Optimization: An Analogy

More time drinking good coffee

7 ☕ vs



Bayesian Optimization: An Analogy

Same idea applies to Bayesian Optimization for Modeling

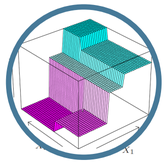
1. Try a few different hyperparameters => see what happens
2. get suggestion on what to try next
3. Now you don't have to train an infinite number of models

Automatic ML Overview

- ~~Feature Preprocessing~~
- ~~Feature Engineering~~
- ~~Hyperparameter Search (part of H2O AutoML)~~
- Ensembles (**part of H2O AutoML**)

Ensembles

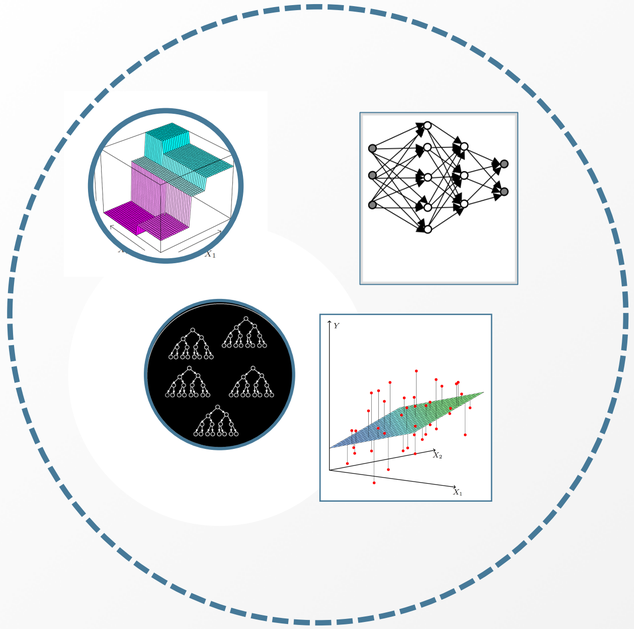
Vanilla Ensembles



Gradient Boosting Machine

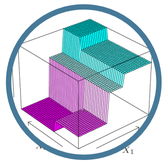
Random Forest

Super Learning Ensembles



Ensembles

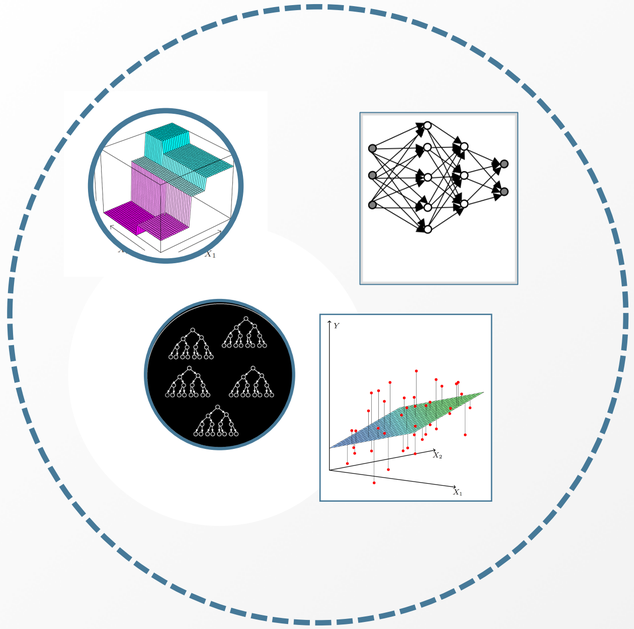
Vanilla Ensembles



Gradient Boosting Machine

Random Forest

(AKA Stacking)



More on Stacked Ensembles

"Stacking is an ensemble procedure where a second-level learner is trained on the output of a collection of base learners."

More on Stacked Ensembles

"Stacking is an ensemble procedure where a **second-level** learner is trained on the output of a collection of base learners."

More on Stacked Ensembles

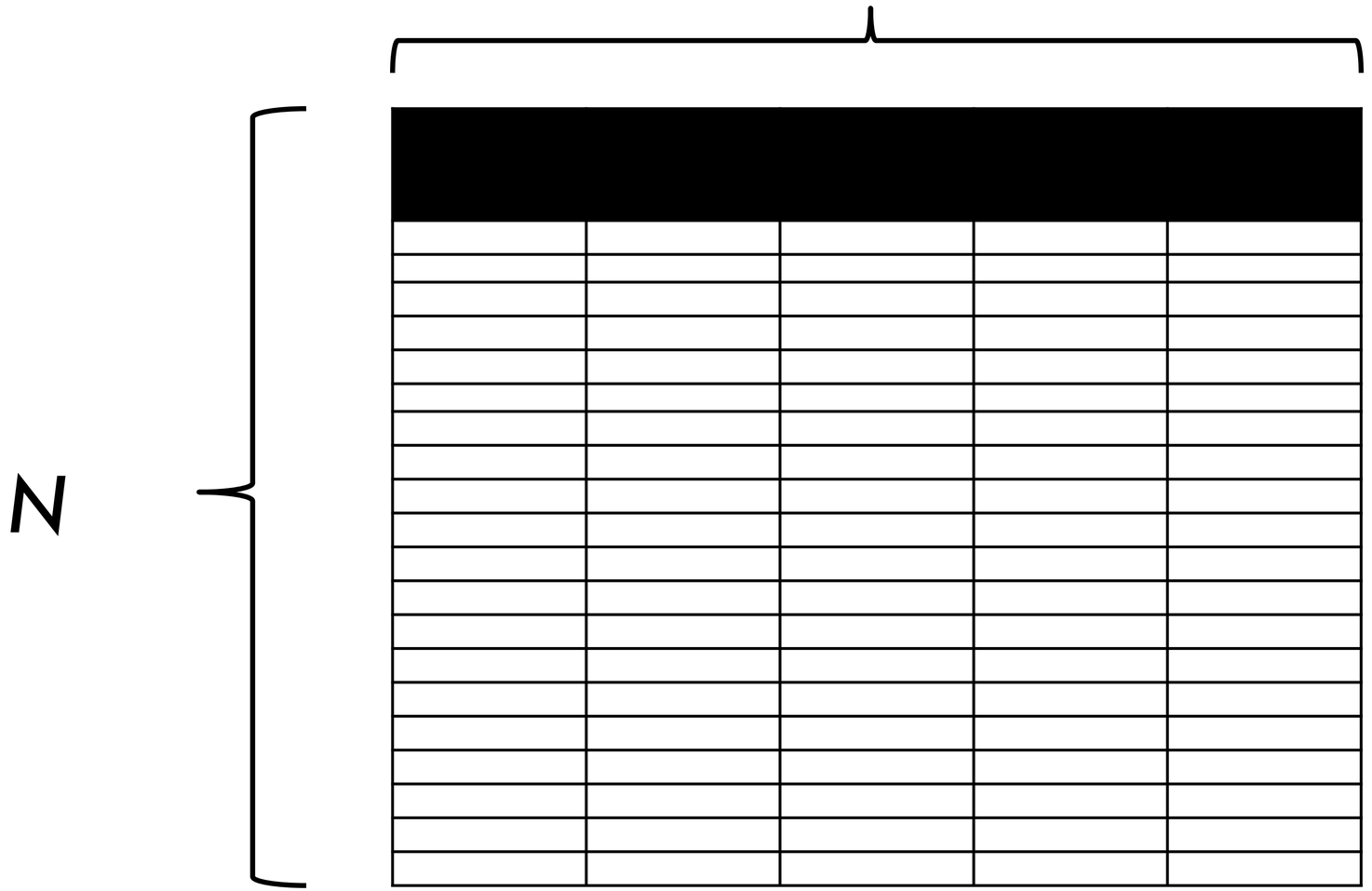
"Stacking is an ensemble procedure where a **metalearner** is trained on the output of a collection of base learners."

More on Stacked Ensembles

"Stacking is an ensemble procedure where a second-level learner is trained on the output of a collection of **base learners**."

Stacked Ensemble Steps

1. **Specify original dataset for training**
2. Specify algorithms with which to train
3. Stack each algo's cross-validated predictions
4. Train final model on cross-validated results



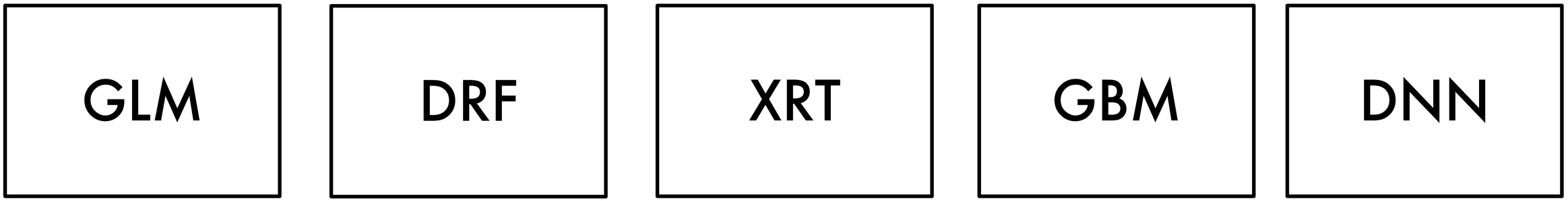
your original training data

"Level-zero" data

Stacked Ensemble Steps

1. Specify original dataset for training
2. **Specify algorithms with which to train**
3. Stack each algo's cross-validated predictions
4. Train final model on cross-validated results

supervised algos used to train



base learners

Stacked Ensemble Steps

1. Specify original dataset for training
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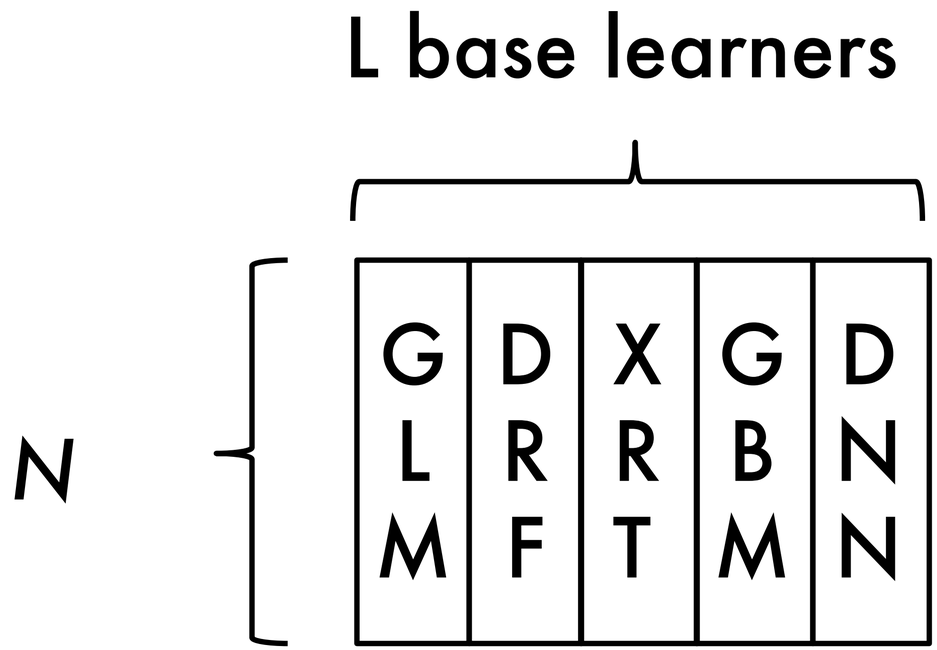
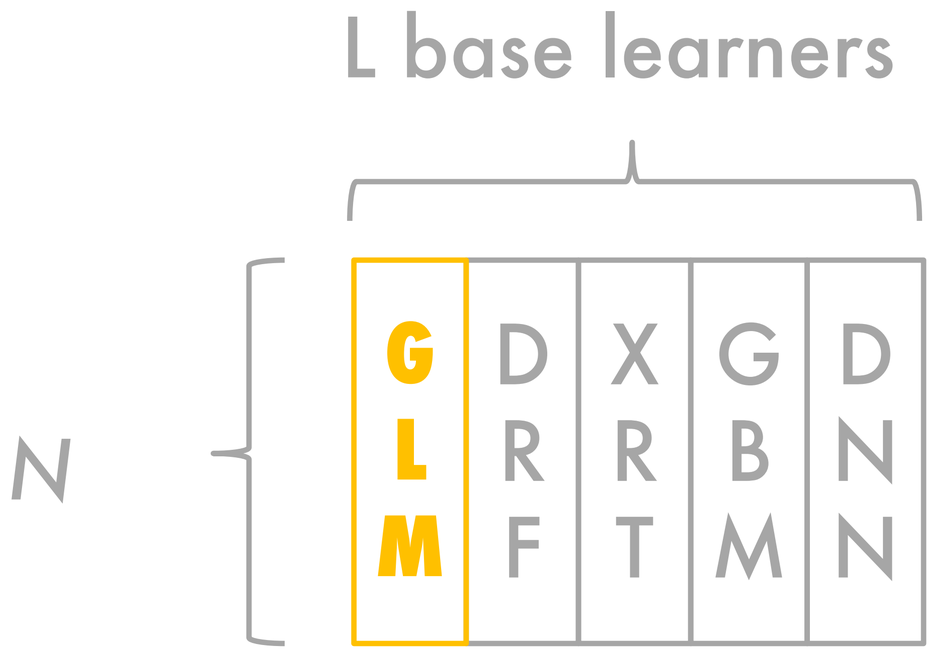
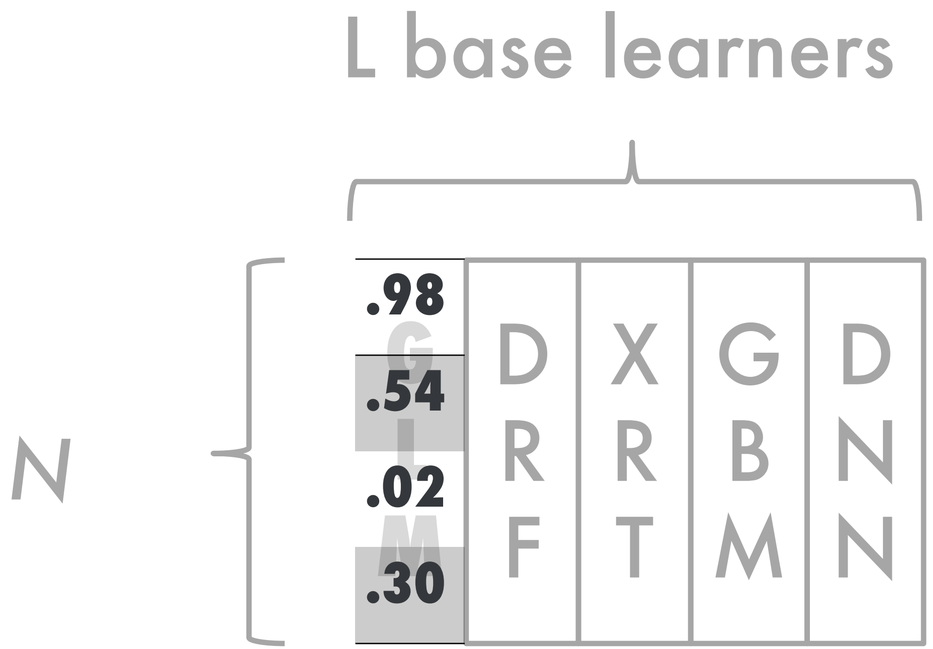
4. Train final model on cross-validated results



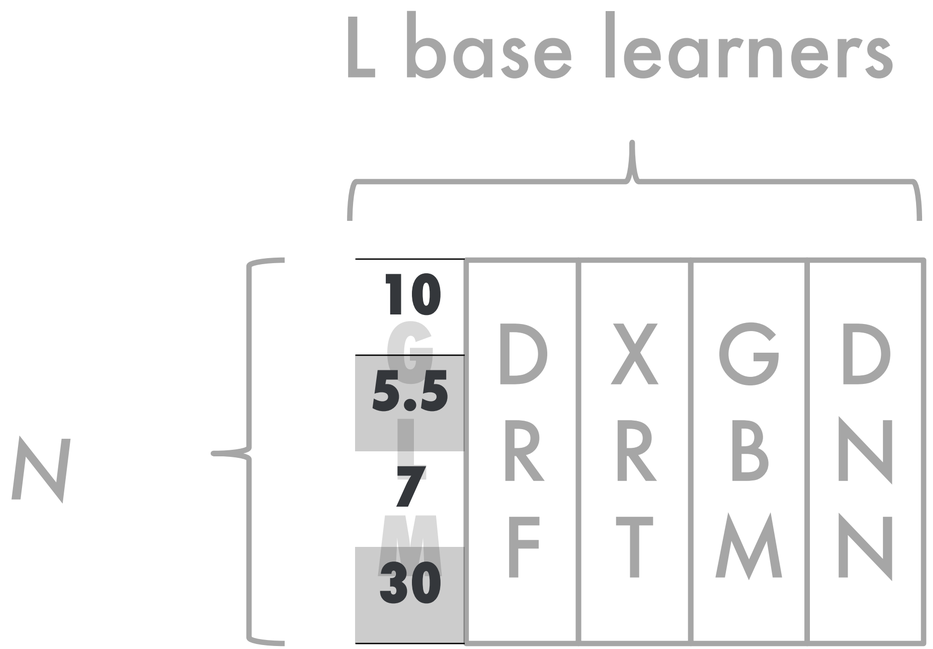
stacking your base learners



meaning:
each column is an algorithm's
cross-validated predictions



meaning:
each column is an algorithm's
cross-validated predictions



meaning:
each column is an algorithm's
cross-validated predictions

How do we get the
cross-validated predictions?

How do we get the cross-validated predictions in H2O?

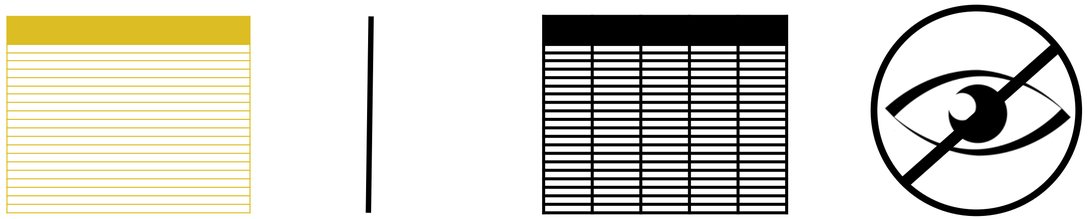
```
keep_cross_validation_predictions =  True
```

what is cross-validation?

quick review

Without K-Fold Cross Validation:

A)

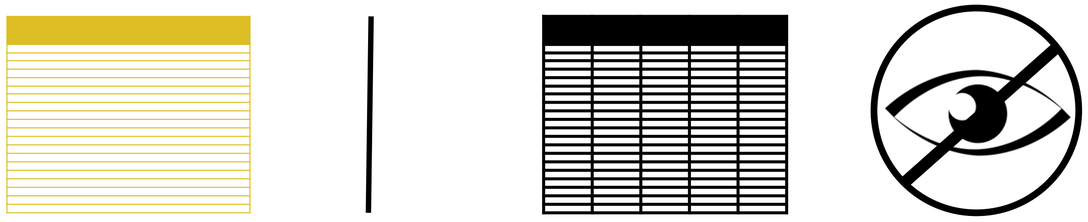


Train

Test

Without K-Fold Cross Validation:

A)

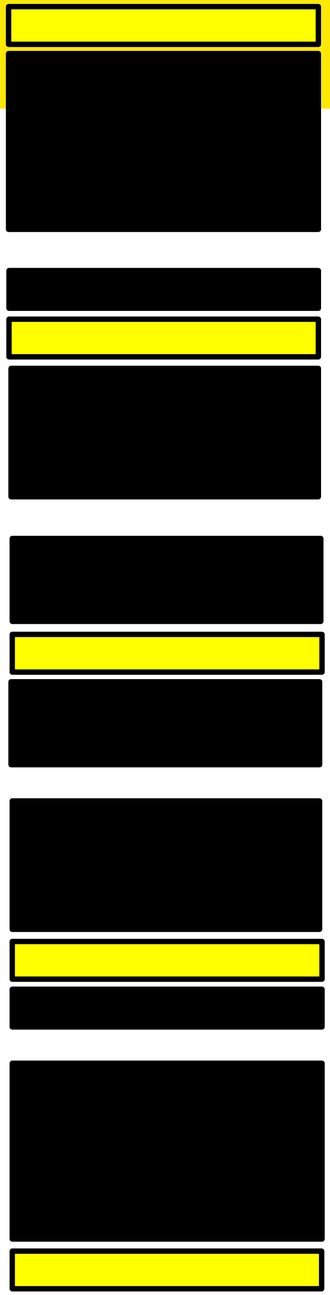


Train | Test

B)

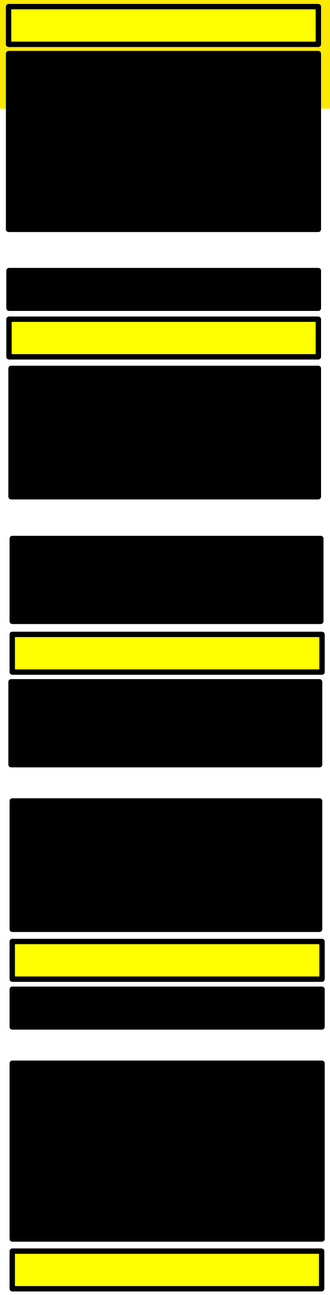
Train | Validate | Test

Model Selection

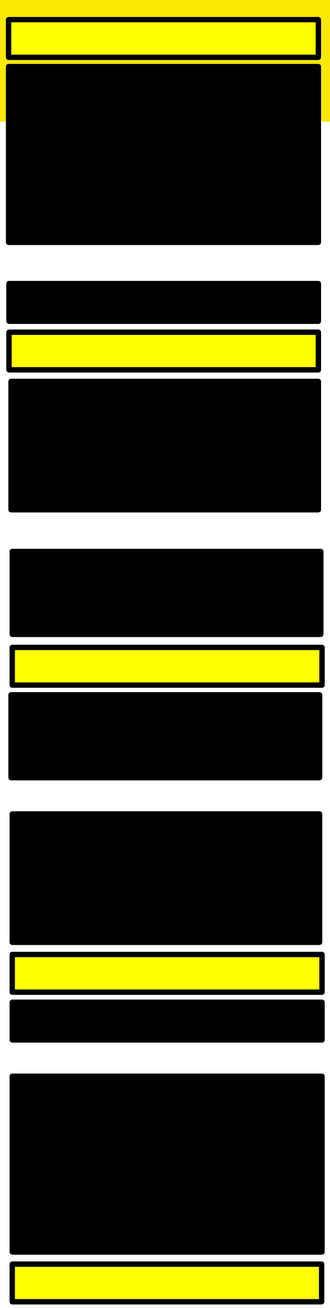


With K-Fold Cross Validation

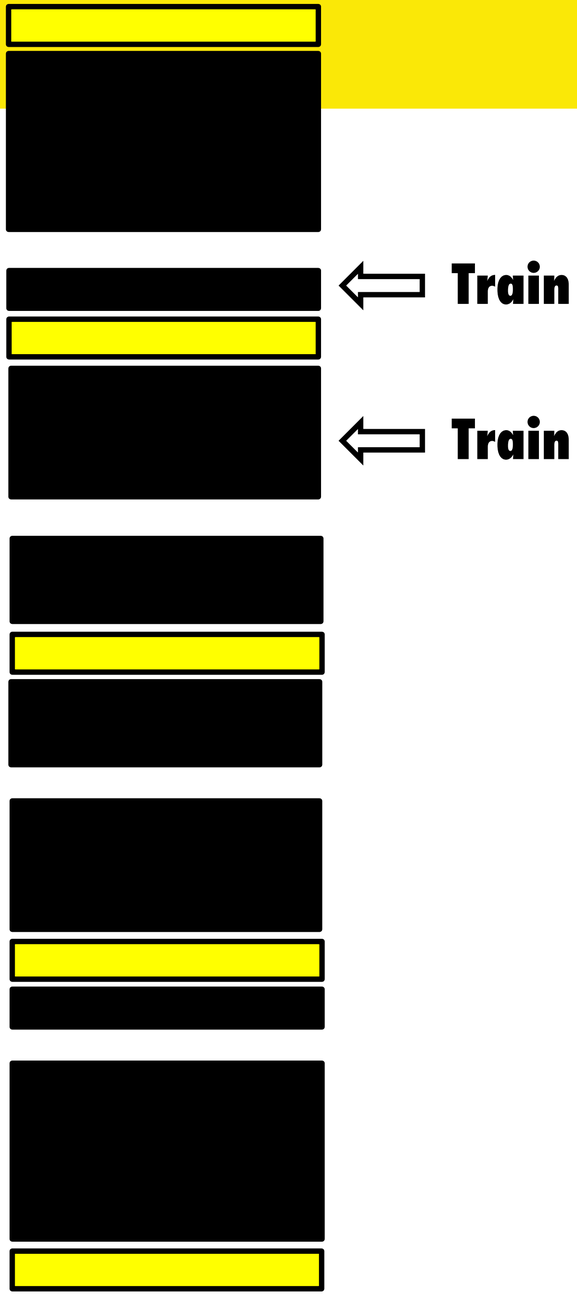
5-fold cross validation
for each algo



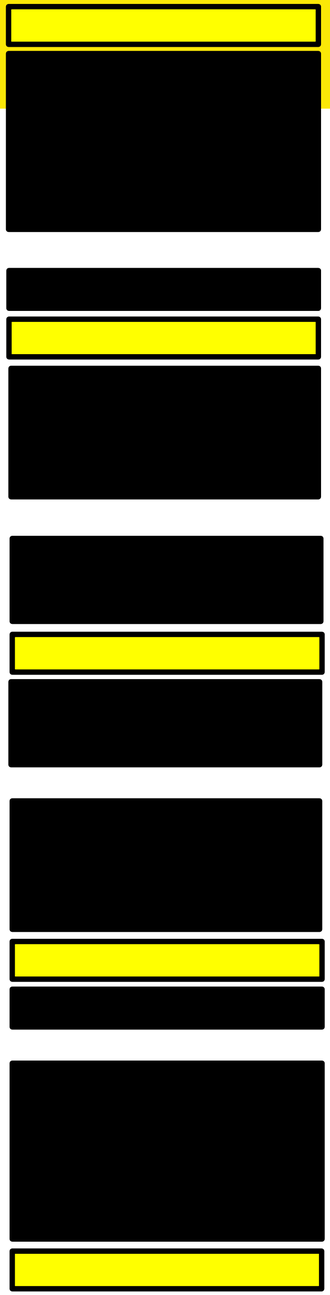
5-fold cross validation for each algo



5-fold cross validation
for each algo

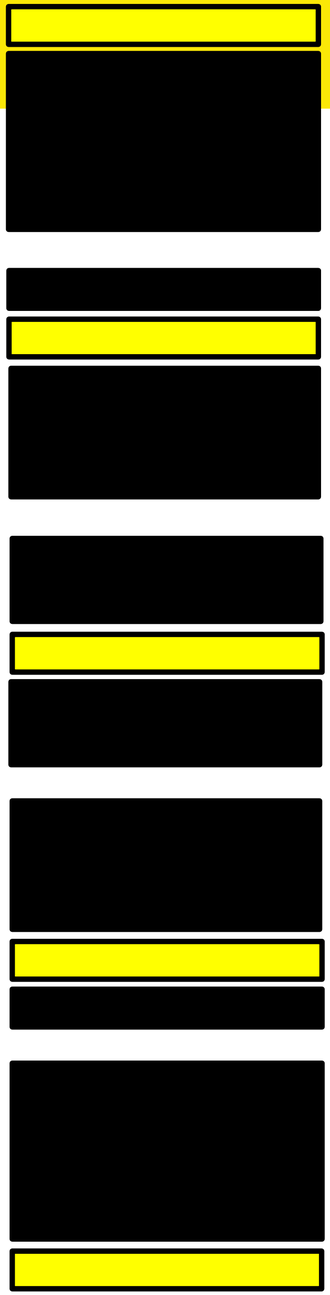


5-fold cross validation for each algo



⇦ **Validate**

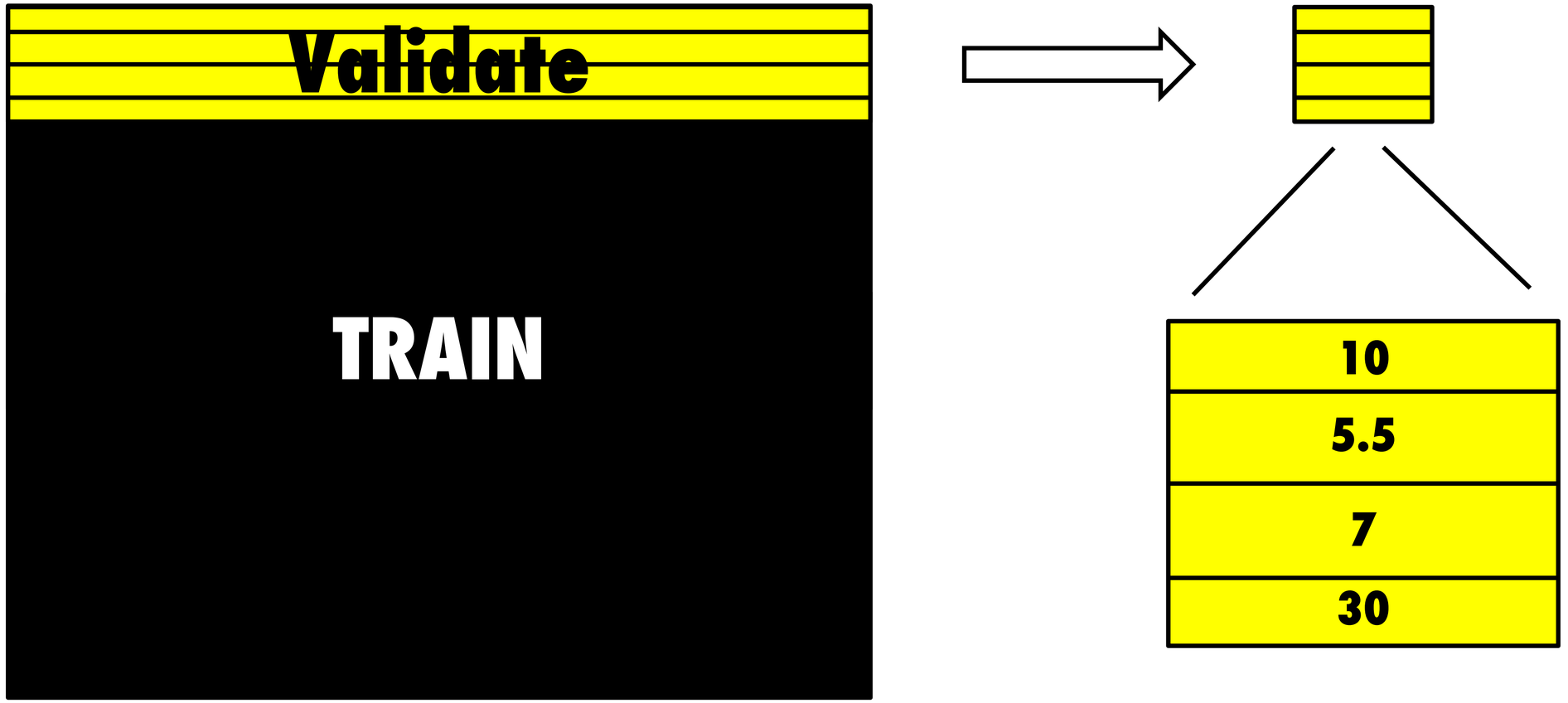
5-fold cross validation for each algo

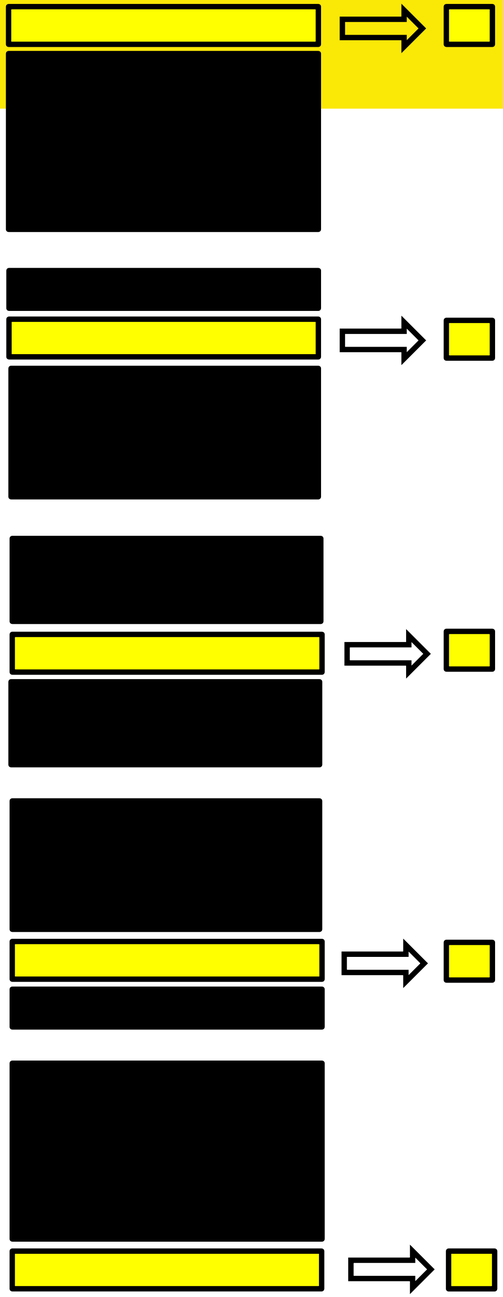


Continue Process

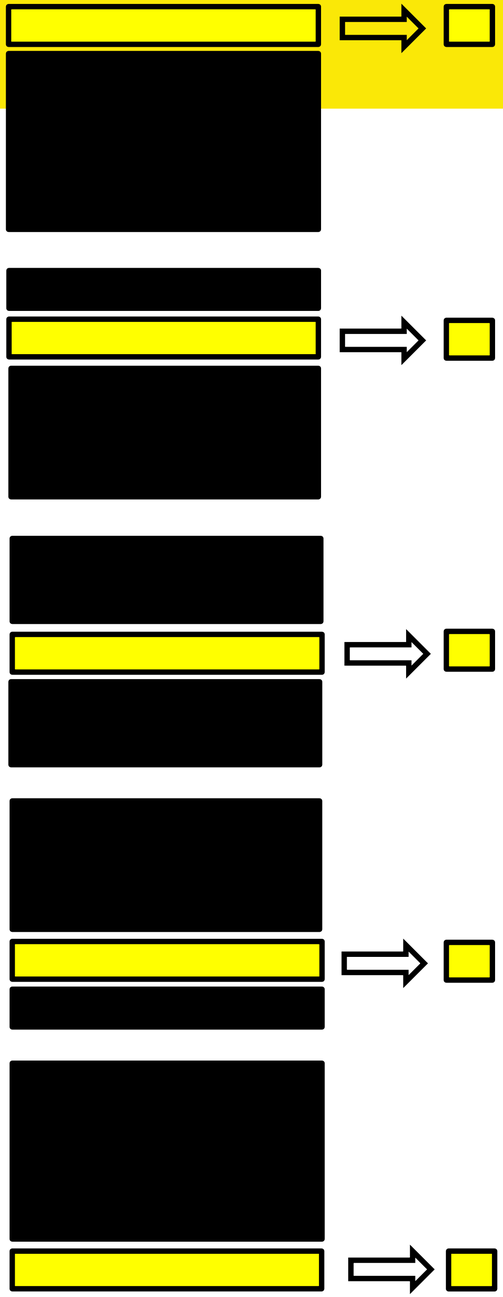
5-fold cross validation for each algo

Cross-Validated Prediction Values

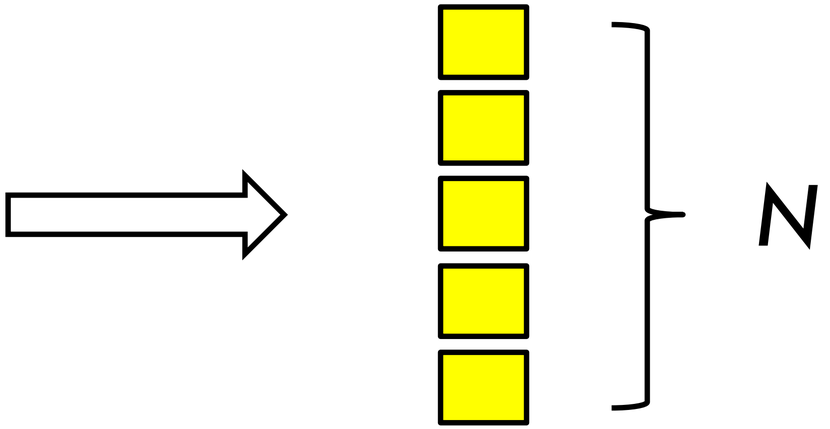




collect the
cross-validated
predictions



collect the cross-validated predictions



Cross-Validation for **Stacking**

K=4

Fold : 1

x0	x1	x2	x3	y
0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

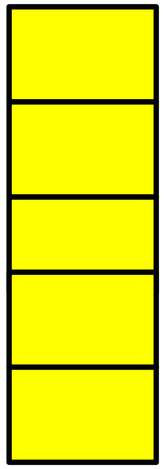
Validate
store pred →

Train

pred
0.96
0.03
0.90
0.12
0.03
0.77
0.08
0.90

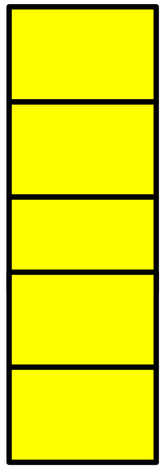
results for each algorithm

DRF



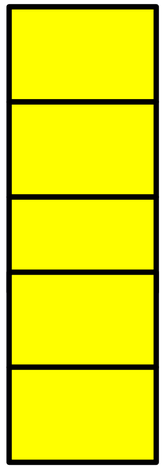
results for each algorithm

XRT

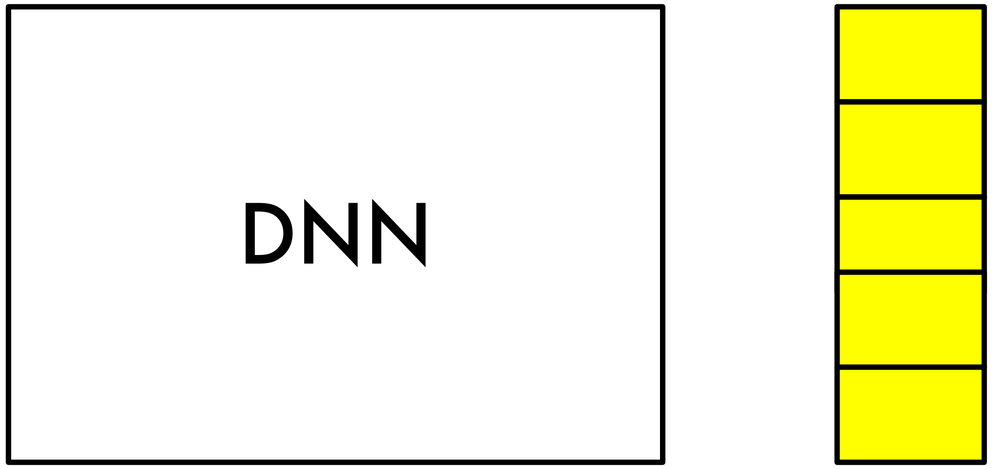


results for each algorithm

GBM



results for each algorithm



results for each algorithm

Stacked Ensemble Steps

1. Specify original dataset for training
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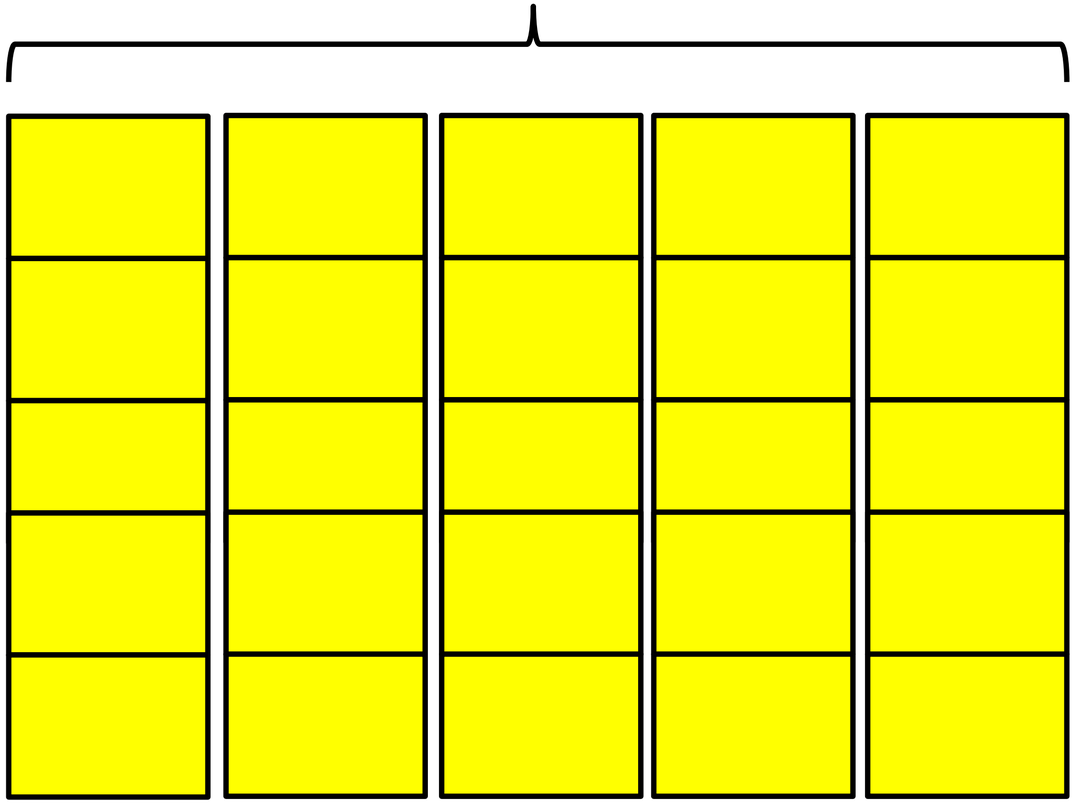
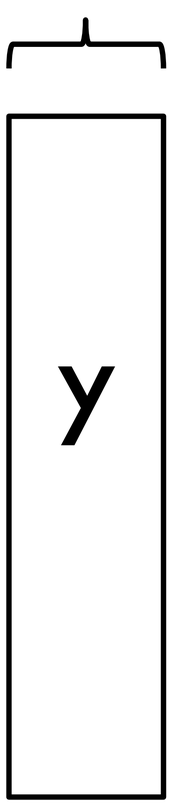
Base Learners' CV Predictions

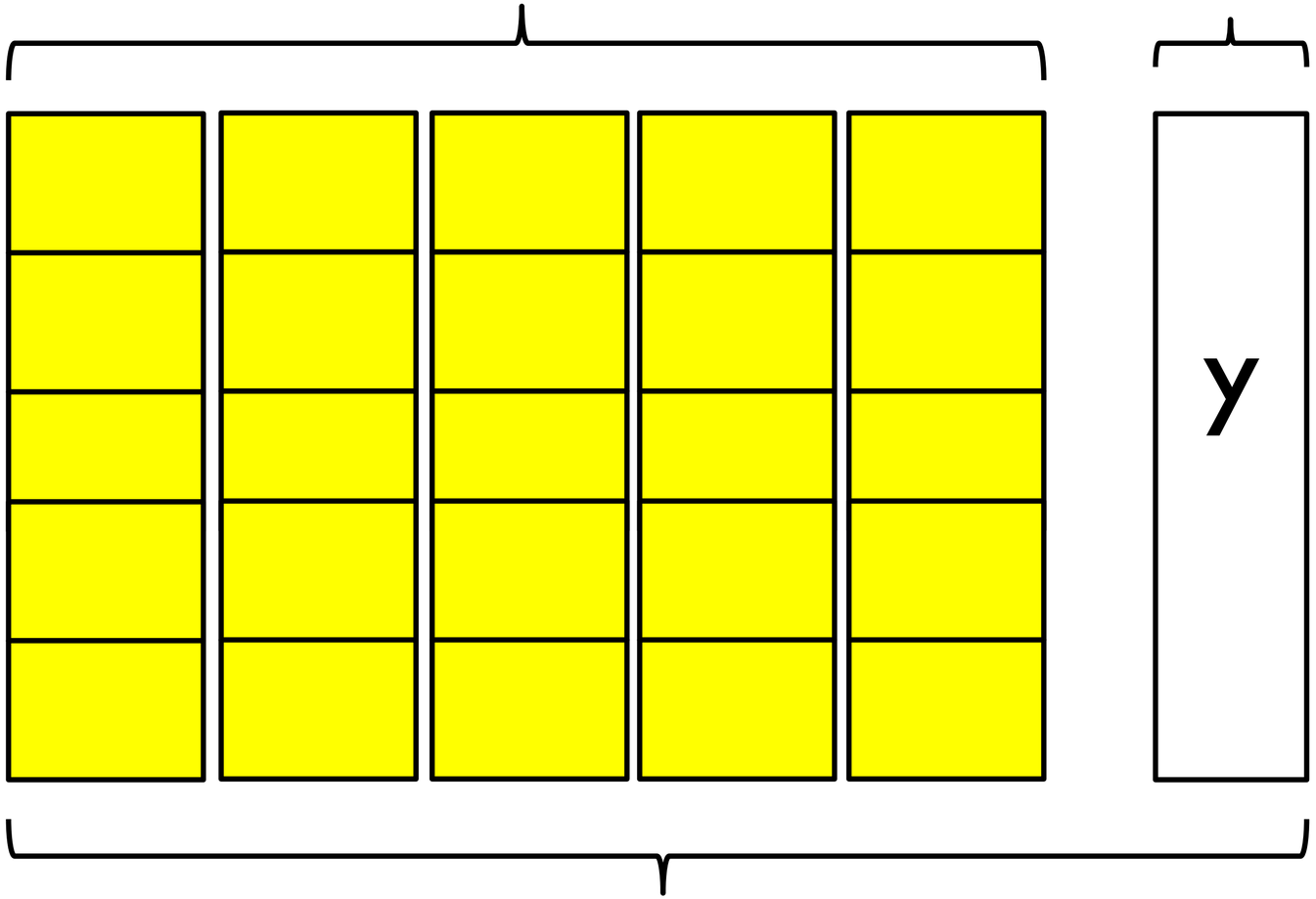


Original Target

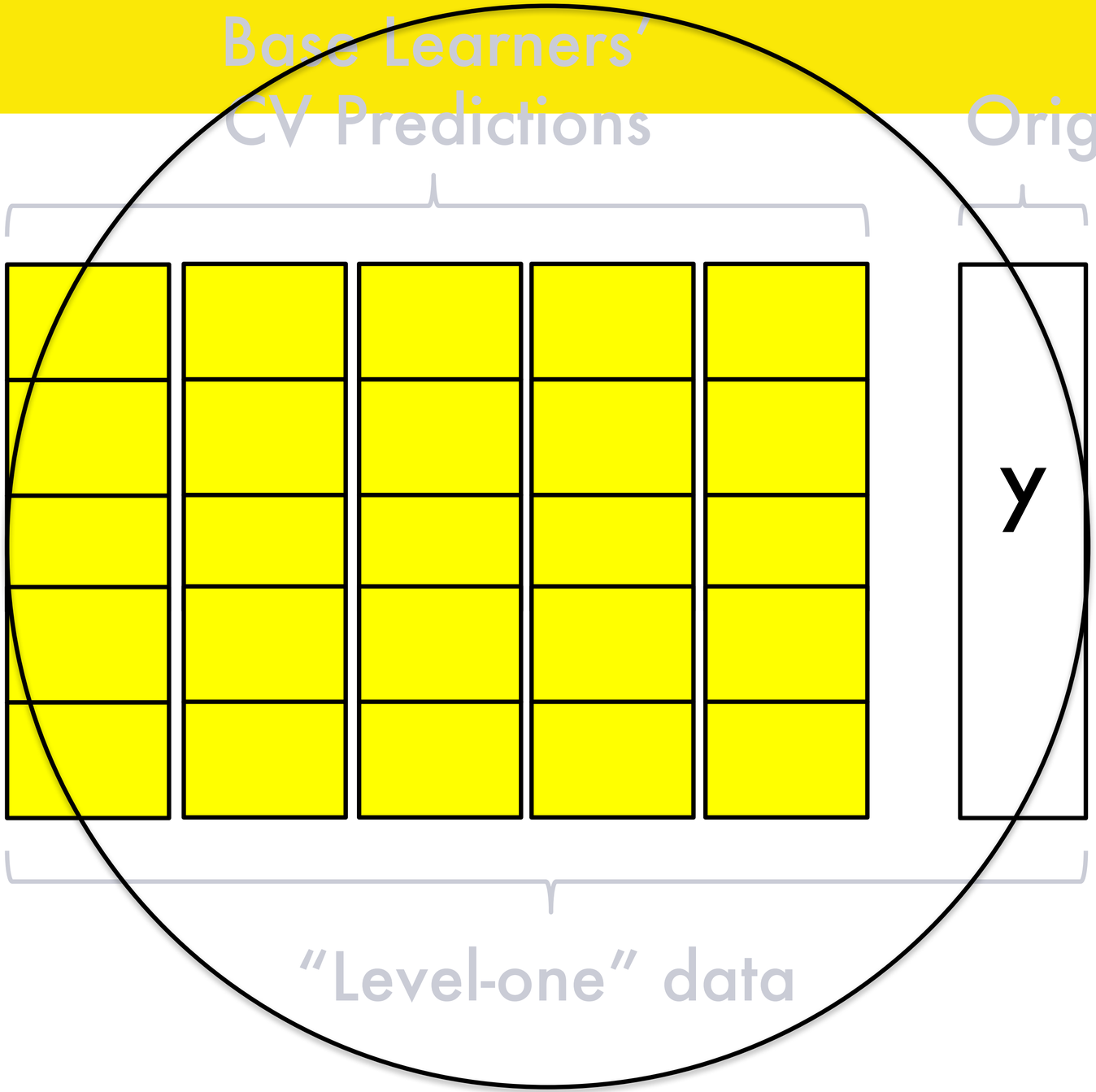


Base Learners'
CV Predictions

Original Target



"Level-one" data



train metalearner on level-one data

train **metalearner**
on level-one data

Random Grid Search & Stacking

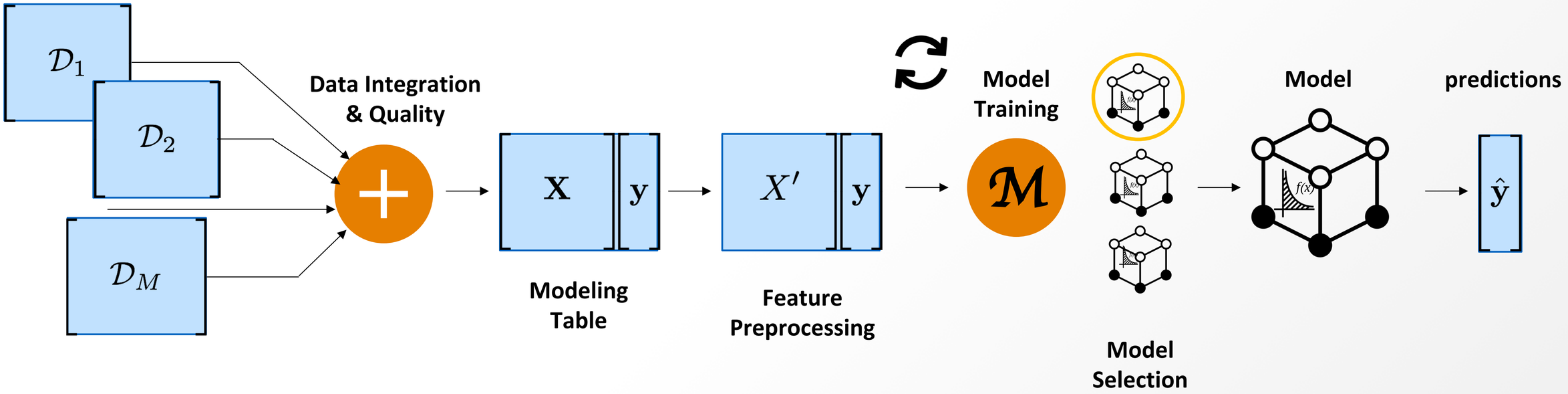
- Random Grid Search combined with Stacked Ensembles is a powerful combination.
- Ensembles perform particularly well if the models they are based on (1) are individually strong, and (2) make uncorrelated errors.
- Stacking uses a second-level metalearning algorithm to find the optimal combination of base learners.

Agenda: Keeping Track

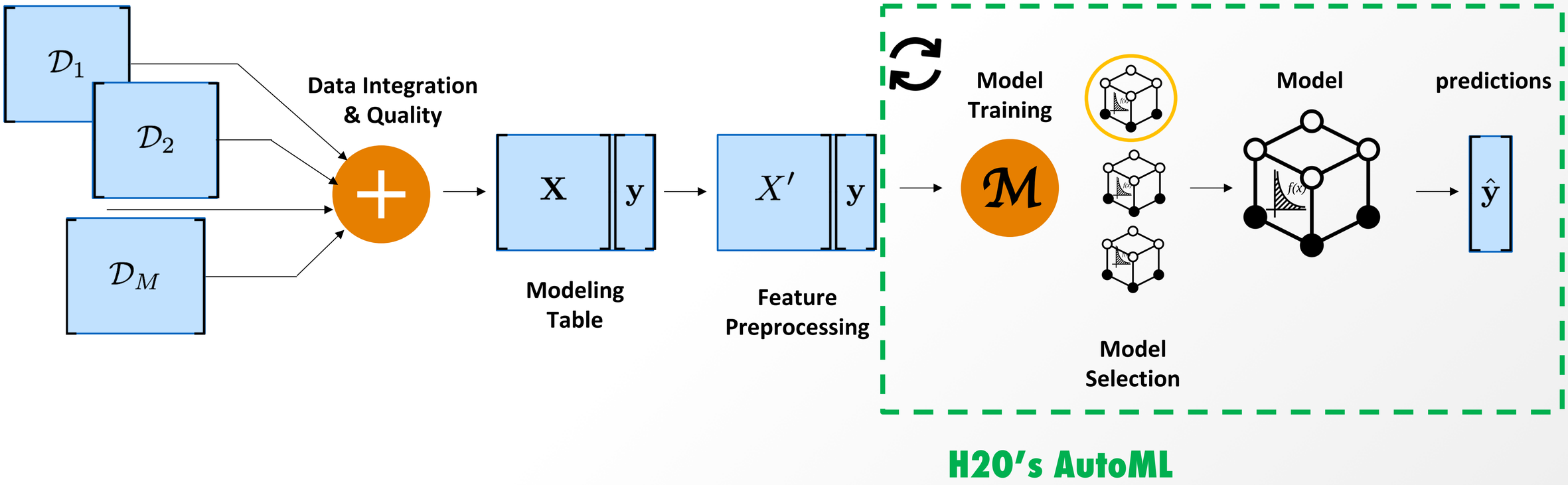
Aspects of Automatic Machine learning:

- ~~Feature Preprocessing~~
- ~~Feature Engineering~~
- ~~Hyperparameter Search~~
- ~~Ensembles~~
- **Up Next: H2O's AutoML**

Updated Machine Learning Pipeline



Updated Machine Learning Pipeline



H2O AutoML (current release)

Data Preprocessing

- Imputation, one-hot encoding, standardization
- Feature selection and/or feature extraction (e.g. PCA)
- Count/Label/Target encoding of categorical features

Model Generation

- Cartesian grid search or random grid search
- Bayesian Hyperparameter Optimization
- Individual models can be tuned using a validation set

Ensembles

- Ensembles often out-perform individual models:
- Stacking / Super Learning (Wolpert, Breiman)
- Ensemble Selection (Caruana)

H2O

H2O AutoML

- Basic data pre-processing (as in all H2O algos).
- Trains a random grid of GBMs, DNNs, GLMs, etc. using a carefully chosen hyper-parameter space
- Individual models are tuned using a validation set.
- Two Stacked Ensembles are trained ("All Models" ensemble & a lightweight "Best of Family" ensemble).
- Returns a sorted "Leaderboard" of all models.

Available in H2O >=3.14

H2O AutoML Interface

- The H2O AutoML interface is designed to have as few parameters as possible so that all the user needs to do is point to their dataset, identify the response column and optionally specify a time constraint or limit on the number of total models trained.
- In both the R and Python API, AutoML uses the same data-related arguments, **x, y, training_frame, validation_frame**, as the other H2O algorithms.
- Most of the time, all you'll need to do is specify the data arguments.
- You can then configure values for **max_runtime_secs and/or max_models** to set explicit time or number-of-model limits on your run

H2O AutoML Interface

- **Required Parameters**
  - **Required Data Parameters**
    - **y**: This argument is the name (or index) of the response column.
    - **training_frame**: Specifies the training set.
  - **Required Stopping Parameters**
    - One of the following stopping strategies (time or number-of-model based) must be specified. When both options are set, then the AutoML run will stop as soon as it hits one of either of these limits.
      - **max_runtime_secs**: This argument controls how long the AutoML run will execute for. This defaults to 3600 seconds (1 hour).
      - **max_models**: Specify the maximum number of models to build in an AutoML run, excluding the Stacked Ensemble models. Defaults to NULL/None

H2O AutoML Interface

- **Optional Parameters**
  - **Optional Data Parameters**
    - **x**: A list/vector of predictor column names or indexes. This argument only needs to be specified if the user wants to exclude columns from the set of predictors. If all columns (other than the response) should be used in prediction, then this does not need to be set.
    - **validation_frame**: This argument is used to specify the validation frame used for early stopping of individual models and early stopping of the grid searches (unless **max_models** or **max_runtime_secs** overrides metric-based early stopping).
    - **leaderboard_frame**: This argument allows the user to specify a particular data frame use to score & rank models on the leaderboard. This frame will not be used for anything besides leaderboard scoring. If a leaderboard frame is not specified by the user, then the leaderboard will use cross-validation metrics instead (or if cross-validation is turned off by setting nfolds = 0, then a leaderboard frame will be generated automatically from the validation frame (if provided) or the training frame).
    - **fold_column**: Specifies a column with cross-validation fold index assignment per observation. This is used to override the default, randomized, 5-fold cross-validation scheme for individual models in the AutoML run.
    - **weights_column**: Specifies a column with observation weights. Giving some observation a weight of zero is equivalent to excluding it from the dataset; giving an observation a relative weight of 2 is equivalent to repeating that row twice. Negative weights are not allowed.
    - **ignored_columns**: (Optional, Python only) Specify the column or columns (as a list/vector) to be excluded from the model. This is the converse of the x argument.

H2O AutoML Interface

- **Optional Miscellaneous Parameters**
  - **nfolds**: Number of folds for k-fold cross-validation of the models in the AutoML run. Defaults to 5. Use 0 to disable cross-validation; this will also disable Stacked Ensembles (thus decreasing the overall best model performance).
  - **stopping_metric**: Specifies the metric to use for early stopping of the grid searches and individual models. Defaults to "AUTO". The available options are:
    - AUTO: This defaults to logloss for classification, deviance for regression
    - deviance
    - logloss
    - mse
    - rmse
    - mae
    - rmsle
    - auc
    - lift_top_group
    - misclassification
    - mean_per_class_error

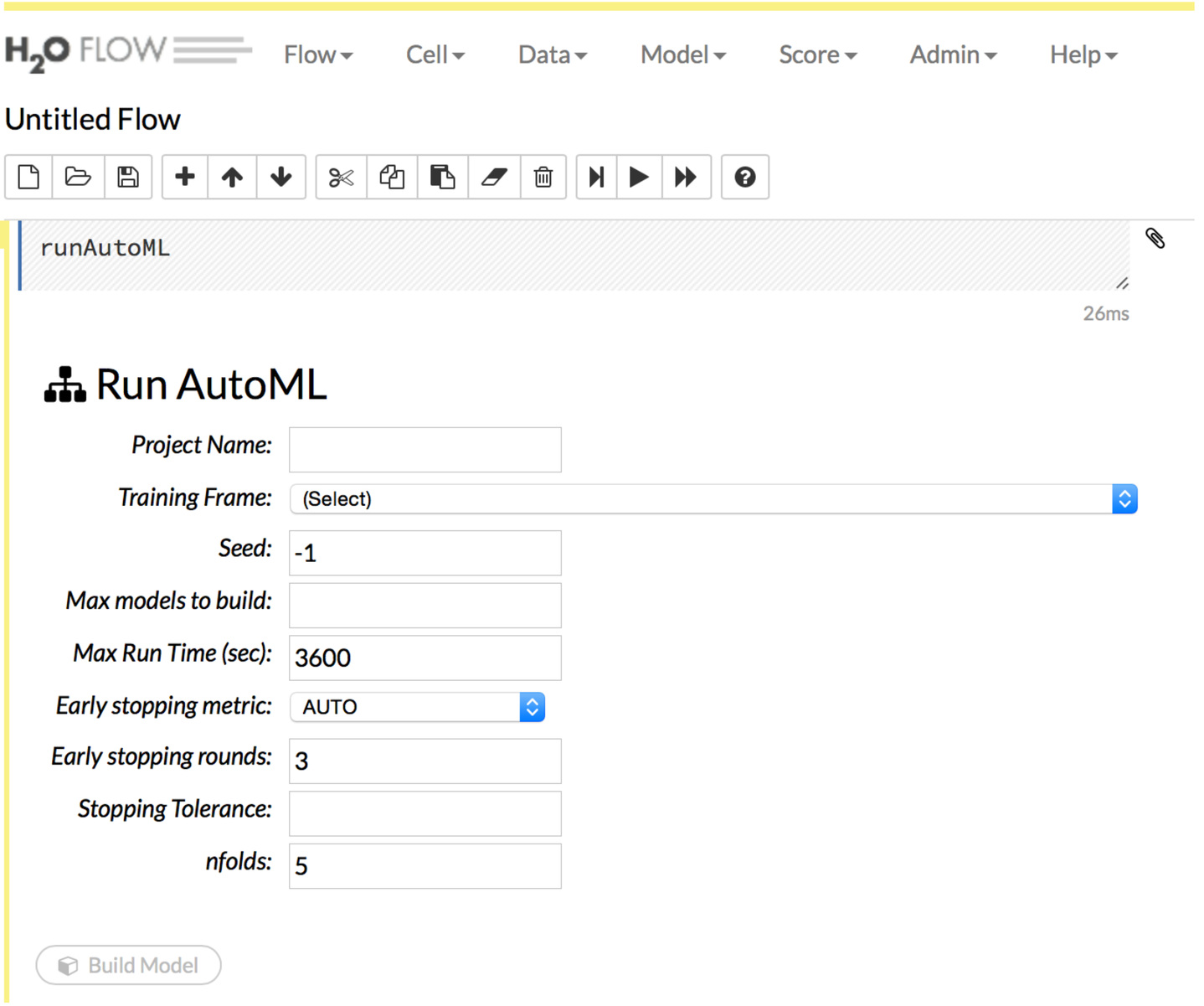
H2O AutoML Interface

- **Optional Miscellaneous Parameters cont.**
  - **stopping_tolerance**: This option specifies the relative tolerance for the metric-based stopping criterion to stop a grid search and the training of individual models within the AutoML run. This value defaults to 0.001 if the dataset is at least 1 million rows; otherwise it defaults to a bigger value determined by the size of the dataset and the non-NA-rate. In that case, the value is computed as 1/sqrt(nrows * non-NA-rate).
  - **stopping_rounds**: This argument is used to stop model training when the stopping metric (e.g. AUC) doesn't improve for this specified number of training rounds, based on a simple moving average. In the context of AutoML, this controls early stopping both within the random grid searches as well as the individual models. Defaults to 3 and must be an non-negative integer. To disable early stopping altogether, set this to 0.
  - **seed**: Integer. Set a seed for reproducibility. AutoML can only guarantee reproducibility if **max_models** is used because **max_runtime_secs** is resource limited, meaning that if the available compute resources are not the same between runs, AutoML may be able to train more models on one run vs another. Defaults to NULL/None.
  - **project_name**: Character string to identify an AutoML project. Defaults to NULL/None, which means a project name will be auto-generated based on the training frame ID. More models can be trained and added to an existing AutoML project by specifying the same project name in muliple calls to the AutoML function (as long as the same training frame is used in subsequent runs).
  - **exclude_algos**: List/vector of character strings naming the algorithms to skip during the model-building phase. An example use is **exclude_algos** = ["GLM", "DeepLearning", "DRF"] in Python or exclude_algos = c("GLM", "DeepLearning", "DRF") in R. Defaults to None/NULL, which means that all appropriate H2O algorithms will be used, if the search stopping criteria allow. The algorithm names are:
    - GLM
    - DeepLearning
    - GBM
    - DRF (This includes both the Random Forest and Extremely-Randomized Trees (XRT) models. Refer to the Extremely Randomized Trees section in the DRF chapter and the histogram_type parameter description for more information.)
    - StackedEnsemble

H2O AutoML Interface

- **Auto-Generated Frames**
  - If the user doesn't specify a **validation_frame**, then one will be created automatically by randomly partitioning the training data. The validation frame is required for early stopping of the individual algorithms, the grid searches and the AutoML process itself.
  - By default, AutoML uses cross-validation for all models, and therefore we can use cross-validation metrics to generate the leaderboard. If the **leaderboard_frame** is explicitly specified by the user, then that frame will be used to generate the leaderboard metrics instead of using cross-validation metrics.
  - For cross-validated AutoML, when the user specifies:
    - **training**: The **training_frame** is split into training (80%) and validation (20%).
    - **training + leaderboard**: The **training_frame** is split into training (80%) and validation (20%).
    - **training + validation**: Leave frames as-is.
    - **training + validation + leaderboard**: Leave frames as-is.
  - If not using cross-validation (by setting **nfolds** = 0) in AutoML, then we need to make sure there is a test frame (aka. the "leaderboard frame") to score on because cross-validation metrics will not be available. So when the user specifies:
    - **training**: The **training_frame** is split into training (80%), validation (10%) and leaderboard/test (10%).
    - **training + leaderboard**: The **training_frame** is split into training (80%) and validation (20%). Leaderboard frame as-is.
    - **training + validation**: The **validation_frame** is split into validation (50%) and leaderboard/test (50%). Training frame as-is.
    - **training + validation + leaderboard**: Leave frames as-is.

H2O AutoML in Flow GUI



H2O AutoML in R

Example

```
library(h2o)

h2o.init()

train <- h2o.importFile("train.csv")


aml <- h2o.automl(y = "response_colname",
                  training_frame = train,
                  max_runtime_secs = 600)

lb <- aml@leaderboard
```

H2O AutoML in Python

Example

```
import h2o

from h2o.automl import H2OAutoML

h2o.init()

train = h2o.import_file("train.csv")

aml = H2OAutoML(max_runtime_secs = 600)
aml.train(y = "response_colname",
          training_frame = train)

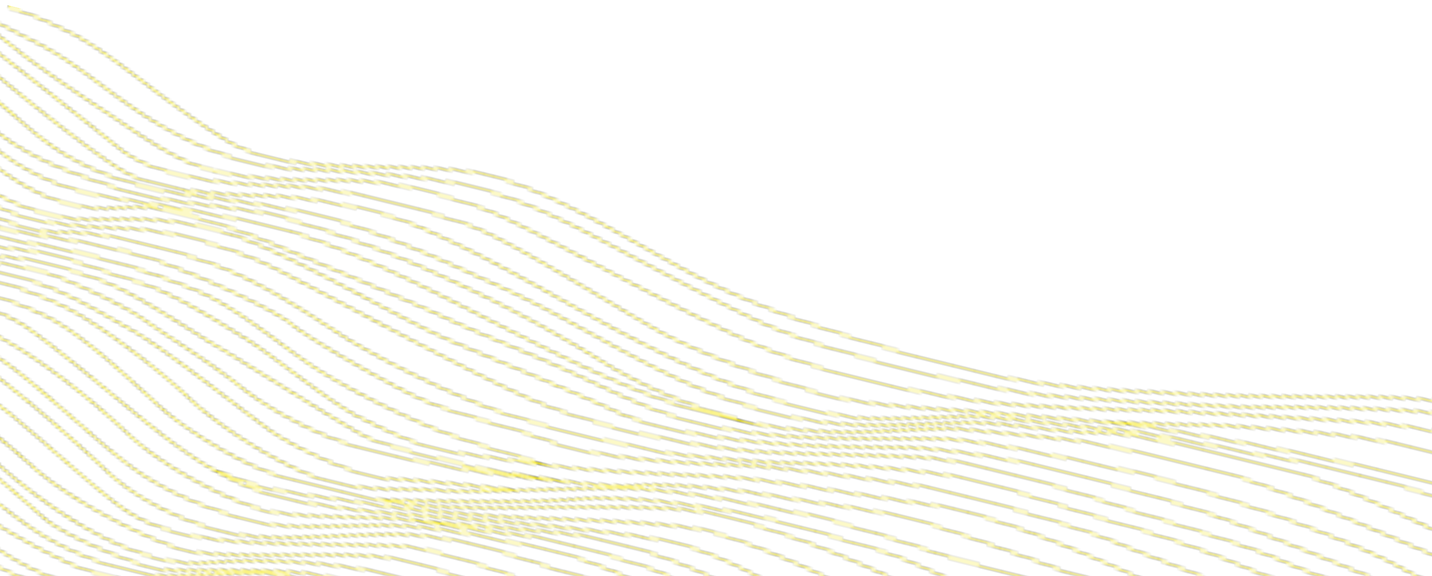
lb = aml.leaderboard
```

H2O AutoML Leaderboard

model_id	auc	logloss
StackedEnsemble_AllModels_0_AutoML_20171121_012135	0.788321	0.554019
StackedEnsemble_BestOfFamily_0_AutoML_20171121_012135	0.783099	0.559286
GBM_grid_0_AutoML_20171121_012135_model_1	0.780554	0.560248
GBM_grid_0_AutoML_20171121_012135_model_0	0.779713	0.562142
GBM_grid_0_AutoML_20171121_012135_model_2	0.776206	0.564970
GBM_grid_0_AutoML_20171121_012135_model_3	0.771026	0.570270
DRF_0_AutoML_20171121_012135	0.734653	0.601520
XRT_0_AutoML_20171121_012135	0.730457	0.611706
GBM_grid_0_AutoML_20171121_012135_model_4	0.727098	0.666513
GLM_grid_0_AutoML_20171121_012135_model_0	0.685211	0.635138

Example Leaderboard for binary classification

AutoML Pro Tips!



Before you press the “red button”

AutoML Pro Tips: Input Frames

- Don't use `leaderboard_frame` unless you really need to; use cross-validation metrics to generate the leaderboard instead (default).
- If you only provide `training_frame`, it will chop off 20% of your data for a validation set to be used in early stopping. To control this proportion, you can split the data yourself and pass a `validation_frame` manually.

AutoML Pro Tips: Exclude Algos

- If you have sparse, wide data (e.g. text), use the `exclude_algos` argument to turn off the tree-based models (GBM, RF).
- If you want tree-based algos only, turn off GLM and DNNs via `exclude_algos`.

AutoML Pro Tips: Time & Model Limits

- AutoML will stop after 1 hour unless you change `max_runtime_secs`.
- Running with `max_runtime_secs` is not reproducible since available resources on a machine may change from run to run. Set `max_runtime_secs` to a big number (e.g. 999999999) and use `max_models` instead.

AutoML Pro Tips: Cluster memory

- Reminder: All H2O models are stored in H2O Cluster memory.
- Make sure to give the H2O Cluster a lot of memory if you're going to create hundreds or thousands of models.
- e.g. `h2o.init(max_mem_size = "80G")`

AutoML Pro Tips: Early Stopping

- If you're expecting more models than are listed in the leaderboard, or the run is stopping earlier than `max_runtime_secs`, this is a result of the default "early stopping" settings.
- To allow more time, increase the number of `stopping_rounds` and/or decrease value of `stopping_tolerance`.

AutoML Pro Tips: Add More Models

- If you want to add (train) more models to an existing AutoML project, just make sure to use the same training set and `project_name`.
- If you set the same seed twice it will give you identical models as the first run (not useful), so change the seed or leave it unset.

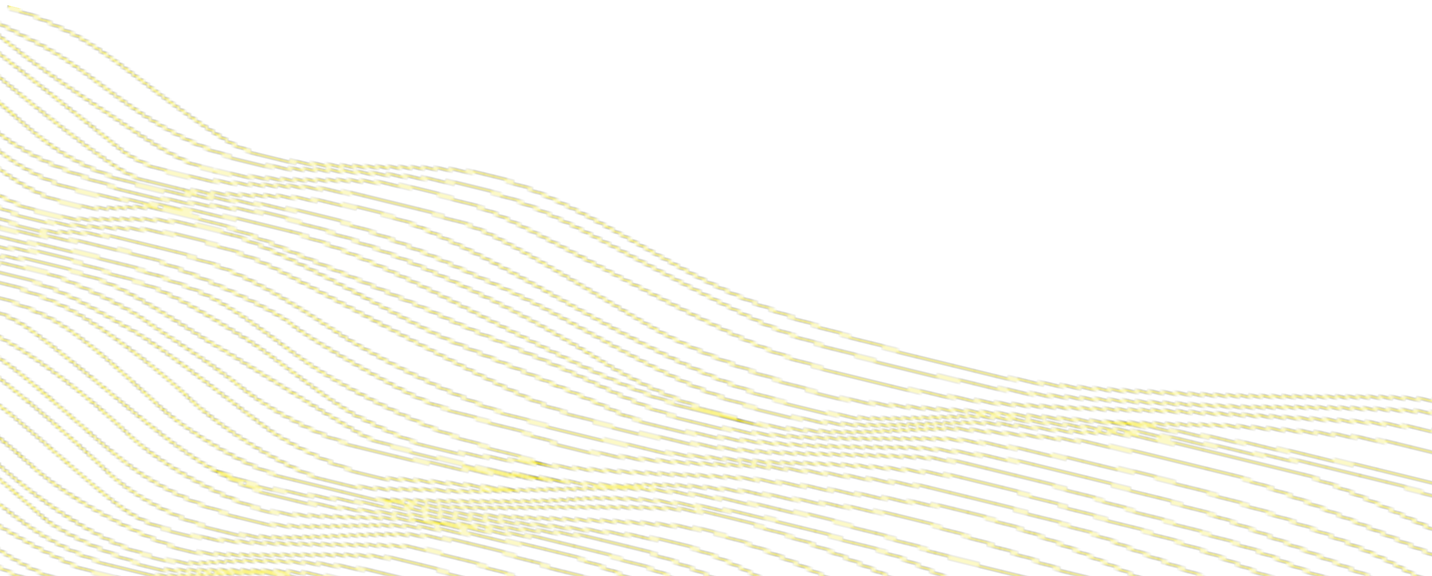
AutoML Pro Tips: Saving Models

- You can save any of the individual models created by the AutoML run. The model ids are listed in the leaderboard.

- If you're taking your leader model (probably a Stacked Ensemble) to production, we'd recommend using "Best of Family" since it only contains 5 models and gets most of the performance of the "All Models" ensemble.

After you press the “red button”

H2O AutoML Demos



H2O AutoML Demos

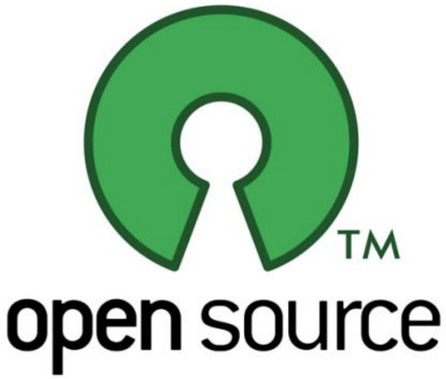
Code available here

https://github.com/navdeep-G/sdss-h2o-automl

H2O Resources

- Documentation: http://docs.h2o.ai
- Tutorials: https://github.com/h2oai/h2o-tutorials
- Slidedecks: https://github.com/h2oai/h2o-meetups
- Videos: https://www.youtube.com/user/0xdata
- Stack Overflow: https://stackoverflow.com/tags/h2o
- Google Group: https://tinyurl.com/h2ostream
- Gitter: http://gitter.im/h2oai/h2o-3
- Events & Meetups: http://h2o.ai/events

Contribute to H2O!



Get in touch over email, Gitter or JIRA.

https://github.com/h2oai/h2o-3/blob/master/CONTRIBUTING.md

Thank you!

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