

# Scalable & Responsible Automatic Machine Learning (AutoML)



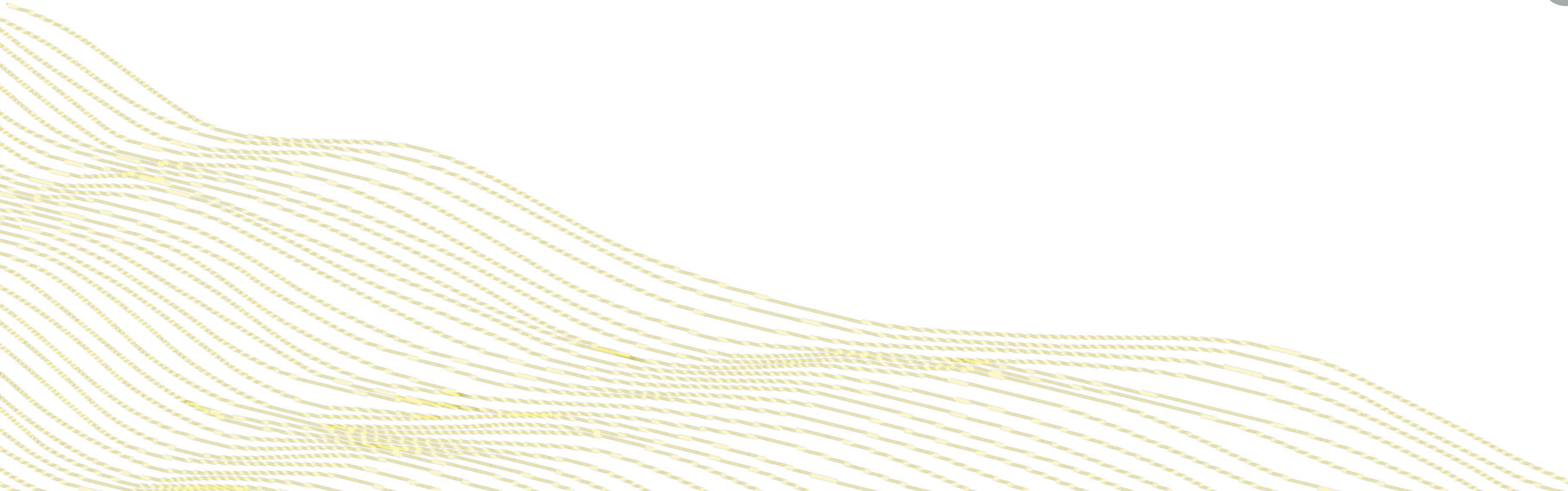
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@ledell

# Agenda

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- Automatic Machine Learning (AutoML)
- H2O AutoML
- Automatic Explainability
- Interpretability & Fairness
- Admissible AutoML

# Intro to Automatic Machine Learning



# Why AutoML?

*“No free lunch”*

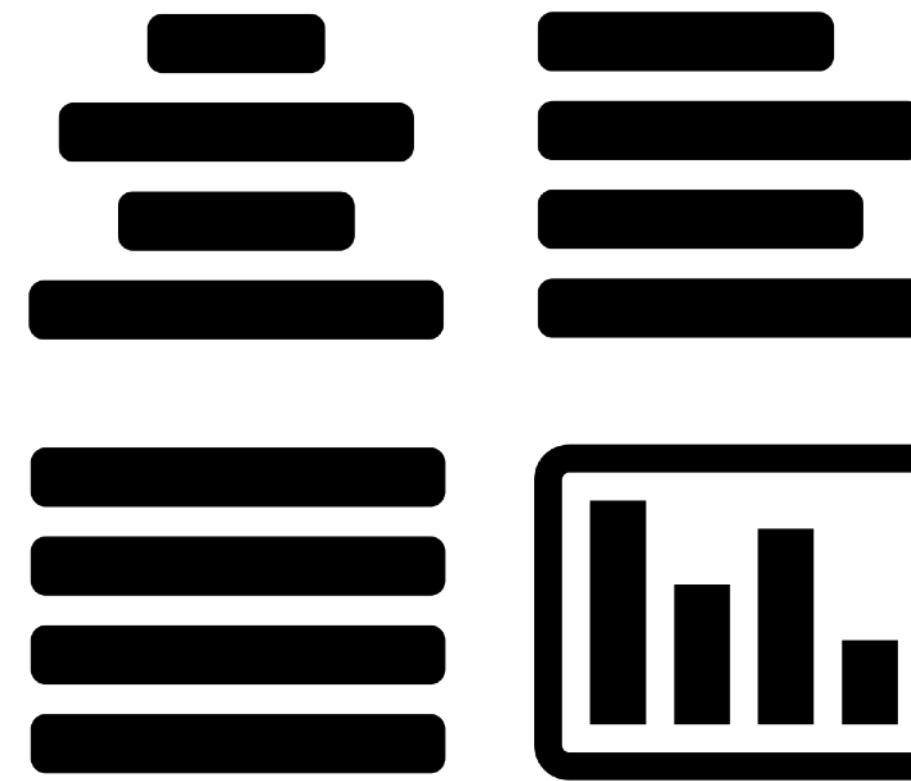
- No Free Lunch Theorem: All algorithms are the equivalent when averaged over all problems. In other words, there's no single “best” algorithm.
- This is why we need to test many algorithms for any particular dataset/problem, and the purpose of AutoML is to automate & speed up this process.

[https://en.wikipedia.org/wiki/No\\_free\\_lunch\\_theorem](https://en.wikipedia.org/wiki/No_free_lunch_theorem)

# Goals & Features of AutoML

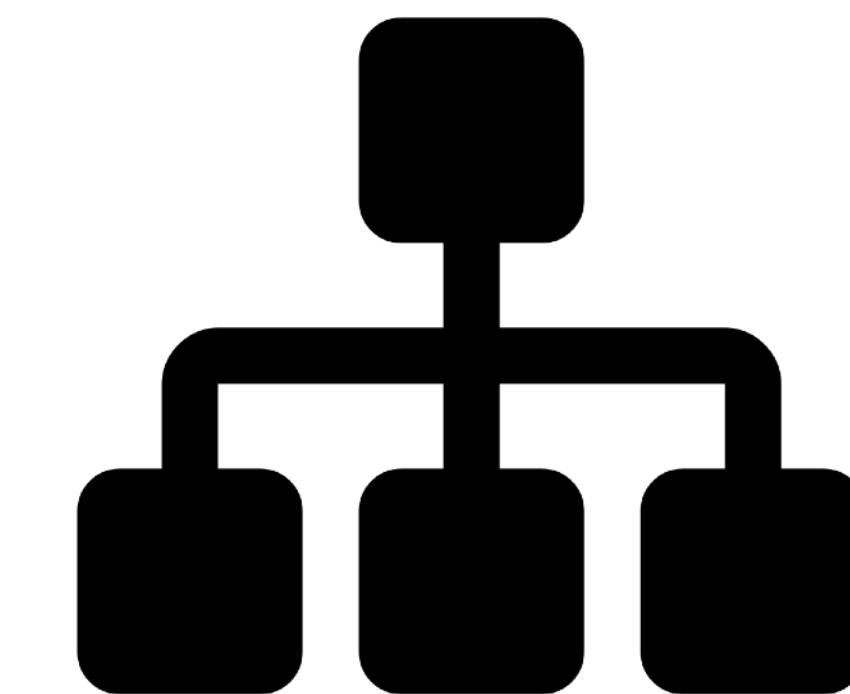
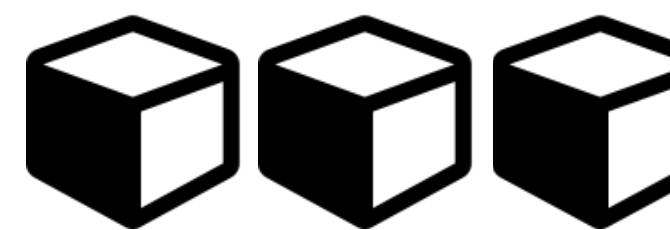
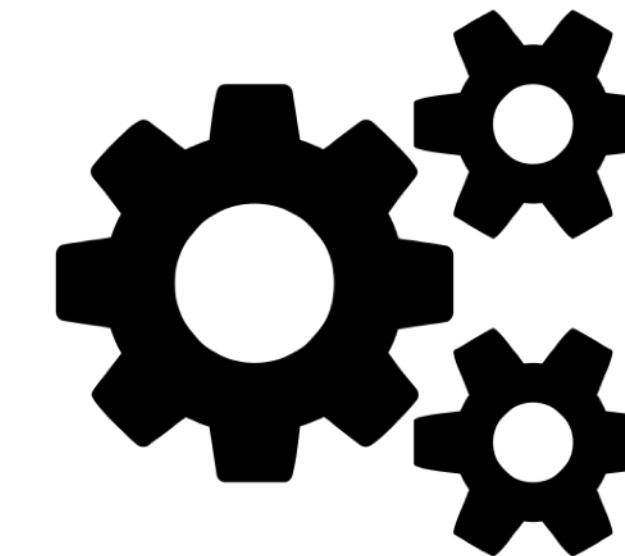
-  Train the best model in the least amount of time.
-  Reduce the human effort & expertise required in machine learning.
-  Improve the performance of machine learning models.
-  Increase reproducibility & establish a baseline for scientific research or applications.

# Aspects of Automatic Machine Learning



Data Prep

Model  
Generation



Ensembles

# Different Flavors of AutoML

The screenshot shows a web browser displaying a blog post from the H2O.ai website. The URL in the address bar is <https://www.h2o.ai/blog/t>. The page title is "The different flavors of AutoML". The post is dated August 15th, 2018. The main image is a black and white photograph of four ice cream cones, each containing a different type of ice cream (vanilla, chocolate, strawberry, and mint chocolate chip). The background of the image features a network of lines and dots, suggesting a data science or machine learning theme.

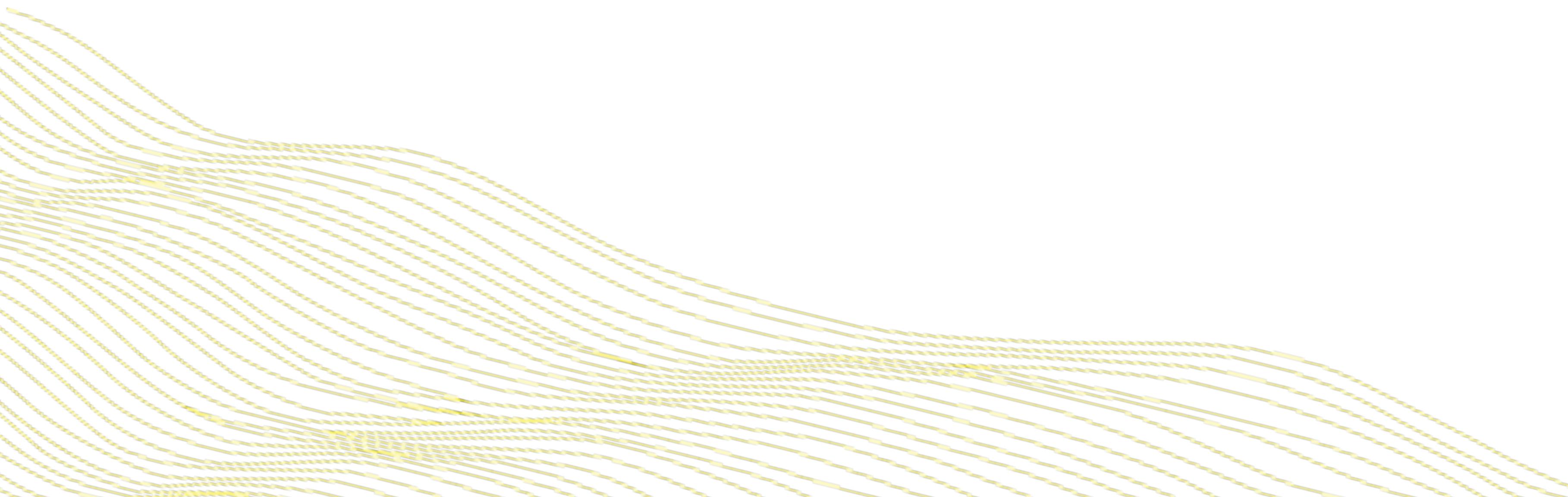
By: Erin LeDell

In recent years, the demand for machine learning experts has outpaced the supply, despite the surge of people entering the field. To address this gap, there have been big strides in the development of user-friendly machine learning software (e.g. [H2O](#), [scikit-learn](#), [keras](#)). Although these tools have made it easy to train and evaluate machine learning models, there is still a good amount of data science knowledge that's required in order to create the *highest-quality* model, given your dataset. Writing the code to perform a hyperparameter search over many different types of algorithms can also be time consuming and repetitive work.

## What is AutoML?

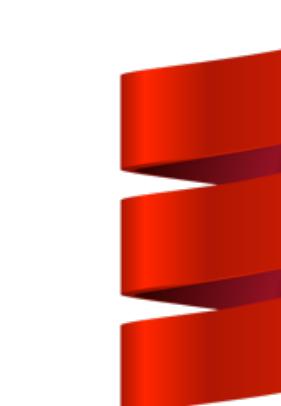
<https://tinyurl.com/flavors-of-automl>

# H2O AutoML



# H2O Machine Learning Platform

- Distributed (multi-core + multi-node) implementations of cutting edge ML algorithms.
- Core algorithms written in high performance Java.
- APIs available in R, Python, Scala; web GUI.
- Easily deploy models to production as pure Java code.
- Works on Hadoop, Spark, EC2, your laptop, etc.



# 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 cross-validation.
- Two Stacked Ensembles are trained (“All Models” ensemble & a lightweight “Best of Family” ensemble).
- Returns a sorted “Leaderboard” of all models.
- All models can be easily exported to production.



# 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 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 Flow (GUI)

**H2O FLOW** Flow ▾ Cell ▾ Data ▾ Model ▾ Score ▾ Admin ▾ Help ▾

Untitled Flow

CS runAutoML 35ms

**Run AutoML**

**PARAMETERS**

project\_name

Optional project name used to group models from multiple AutoML runs into a single Leaderboard; derived from the training data name if not specified.

training\_frame\*

ID of the training data frame.

response\_column\*

Response column

validation\_frame

ID of the validation data frame (used for early stopping in grid searches and for early stopping of the AutoML process itself).

blending\_frame

ID of the H2OFrame used to train the metalearning algorithm in Stacked Ensembles (instead of relying on cross-validated predicted values). When provided, it is also recommended to disable cross validation by setting "nfolds=0" and to provide a leaderboard frame for scoring purposes.

leaderboard\_frame

ID of the leaderboard data frame (used to score models and rank them on the AutoML Leaderboard).

**ADVANCED**

nfold 5

Number of folds for k-fold cross-validation (defaults to 5, must be >=2 or use 0 to disable). Disabling prevents Stacked Ensembles from being built.

balance\_classes

Balance training data class counts via over/under-sampling (for imbalanced data).

fold\_column

Fold column (contains fold IDs) in the training frame. These assignments are used to create the folds for cross-validation of the models.

weights\_column

Weights column in the training frame, which specifies the row weights used in model training.

sort\_metric AUTO

Metric used to sort leaderboard

exclude\_algos Search...  
 GLM  
 DRF  
 GBM  
 DeepLearning  
 StackedEnsemble  
 XGBoost

A list of algorithms to skip during the model-building phase.

**OUTLINE FLOWS CLIPS HELP**

Help

Using Flow for the first time?  
[Quickstart Videos](#)

Or, [view example Flows](#) to explore and learn H2O.

STAR H2O ON GITHUB!  
[Star](#)

GENERAL

- Flow Web UI ...
  - ... Importing Data
  - ... Building Models
  - ... Making Predictions
  - ... Using Flows
  - ... Troubleshooting Flow

EXAMPLES

Flow packs are a great way to explore and learn H2O. Try out these Flows and run them in your browser.  
[Browse installed packs...](#)

H2O REST API

- Routes
- Schemas

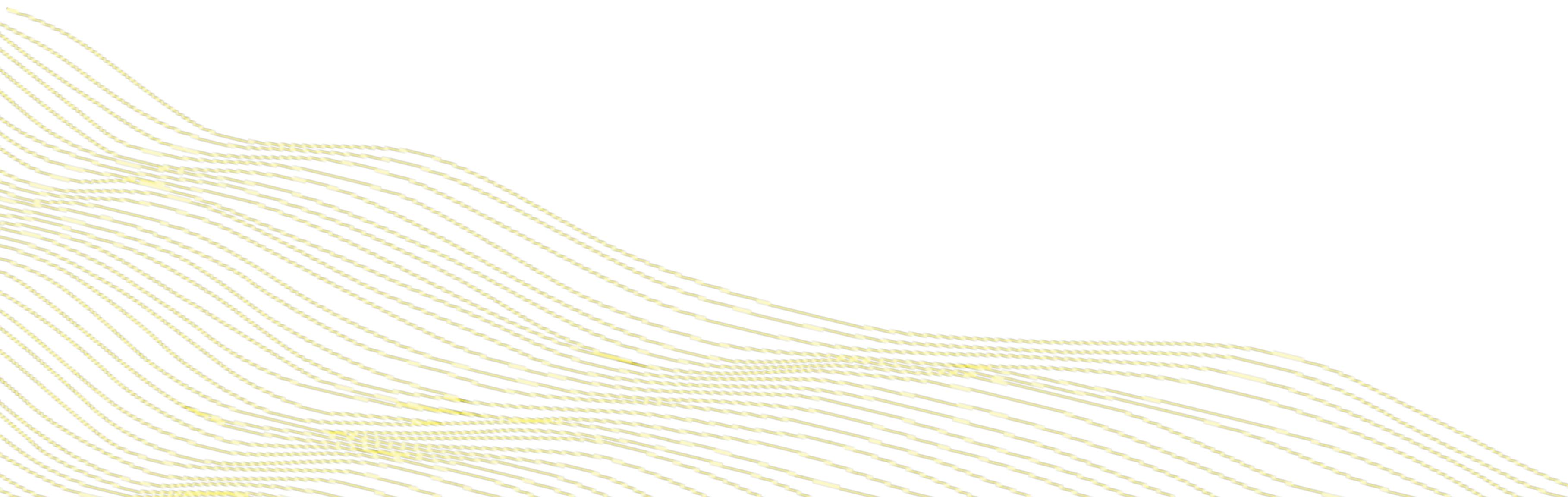
# H2O AutoML Leaderboard

▲	model_id	auc	logloss	aucpr	mean_per_class_error	rmse	mse
1	StackedEnsemble_AllModels_AutoML_20200709_004...	0.8378355	0.2866370	0.4481733	0.2498460	0.2913039	0.08485799
2	StackedEnsemble_BestOfFamily_AutoML_20200709_0...	0.8369381	0.2869531	0.4462222	0.2500683	0.2914670	0.08495302
3	XGBoost_3_AutoML_20200709_004415	0.8366588	0.2809896	0.4502926	0.2552901	0.2894478	0.08378002
4	GBM_4_AutoML_20200709_004415	0.8330289	0.2848382	0.4239271	0.2593298	0.2919957	0.08526147
5	GBM_3_AutoML_20200709_004415	0.8325824	0.2852444	0.4195761	0.2552272	0.2922670	0.08542002
6	GBM_2_AutoML_20200709_004415	0.8323248	0.2855498	0.4185351	0.2589230	0.2924915	0.08555129
7	GBM_1_AutoML_20200709_004415	0.8322315	0.2855884	0.4200573	0.2622791	0.2922375	0.08540278
8	XGBoost_1_AutoML_20200709_004415	0.8317490	0.2858897	0.4326282	0.2618297	0.2923182	0.08544993
9	GBM_5_AutoML_20200709_004415	0.8296069	0.2874258	0.4040567	0.2569593	0.2938664	0.08635746
10	XGBoost_2_AutoML_20200709_004415	0.8277037	0.2899311	0.4265391	0.2624847	0.2943874	0.08666391
11	DRF_1_AutoML_20200709_004415	0.8120043	0.3008964	0.3722857	0.2731671	0.2991530	0.08949252
12	GLM_1_AutoML_20200709_004415	0.6873574	0.3510707	0.2172795	0.3673990	0.3194751	0.10206432



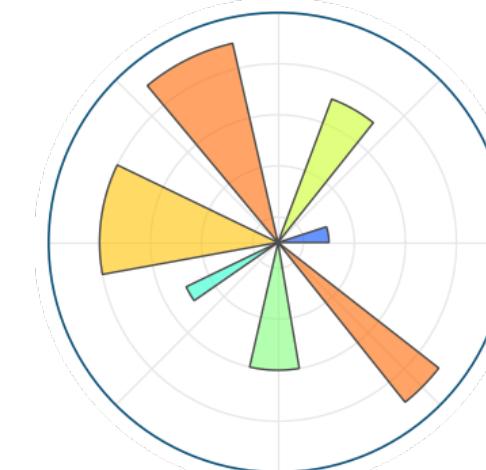
Example Leaderboard for binary classification

# Auto Explainability



# H2O AutoML Explainability

- The new `h2o.explain()` interface automatically generates many explanations (annotated visualizations) for a single model or a group of models (e.g. AutoML leaderboard).
- Row-wise explanations are available via the `h2o.explain_row()` companion function.
- Visualizations are created with `ggplot2` in R and `matplotlib` in Python, and can be customized.



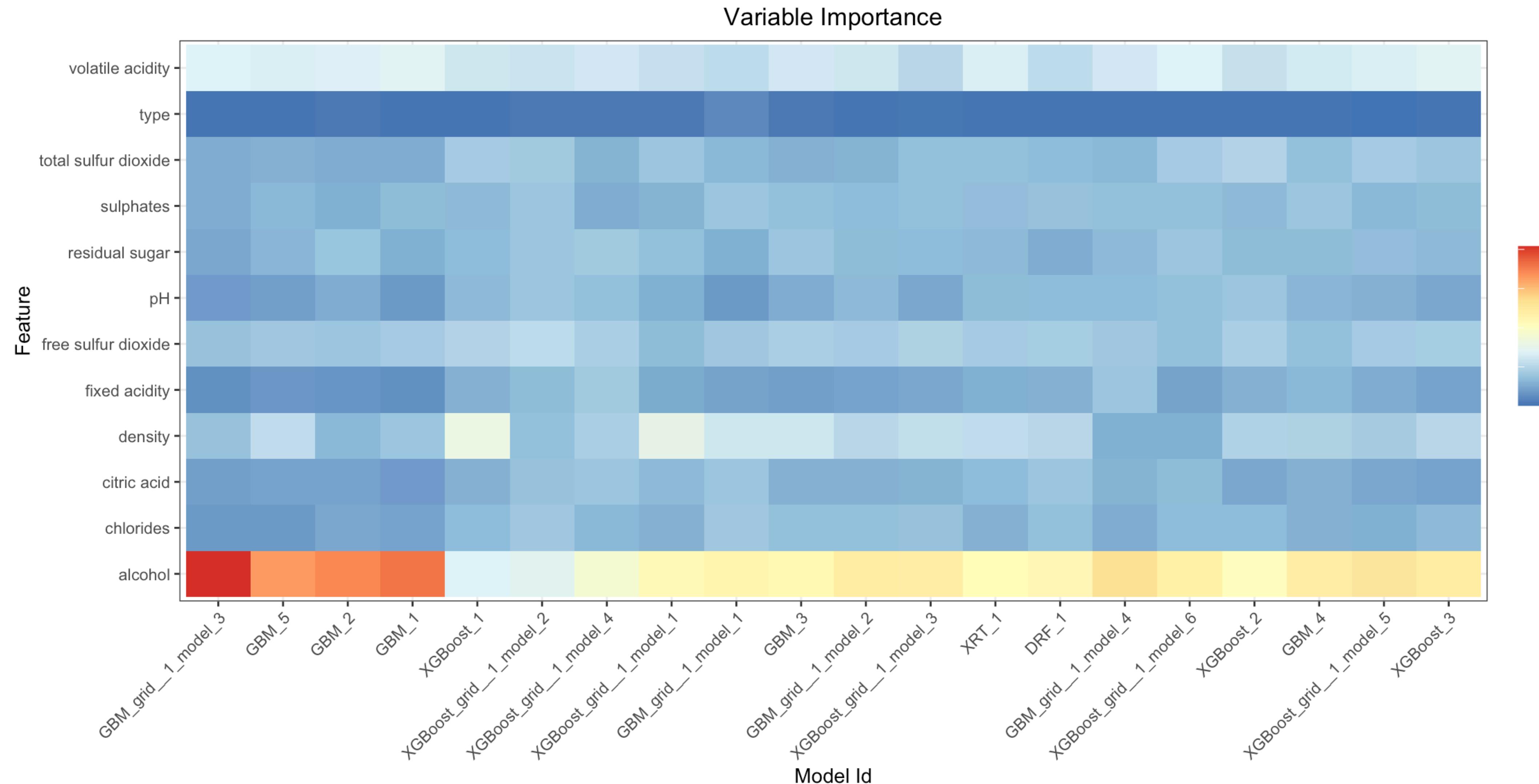
# H2O AutoML Explainability

## Automatic Explanations:

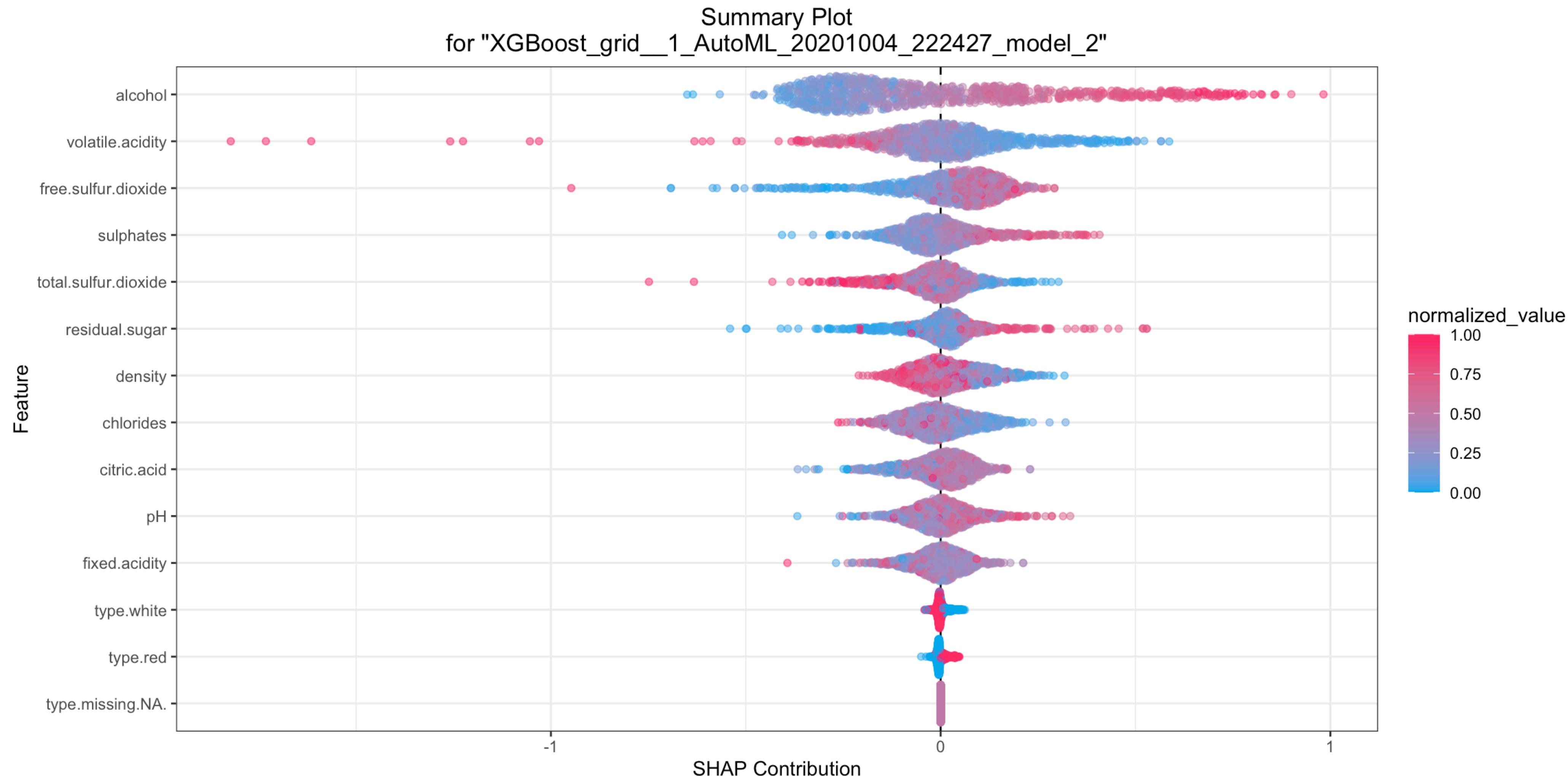


- Variable importance comparisons
- Model correlation heatmap
- SHAP contributions for tree-based models
- Partial dependence (PD) plots
- Individual Conditional Expectation (ICE) plots
- Residual Analysis

# Variable Importance Heatmap

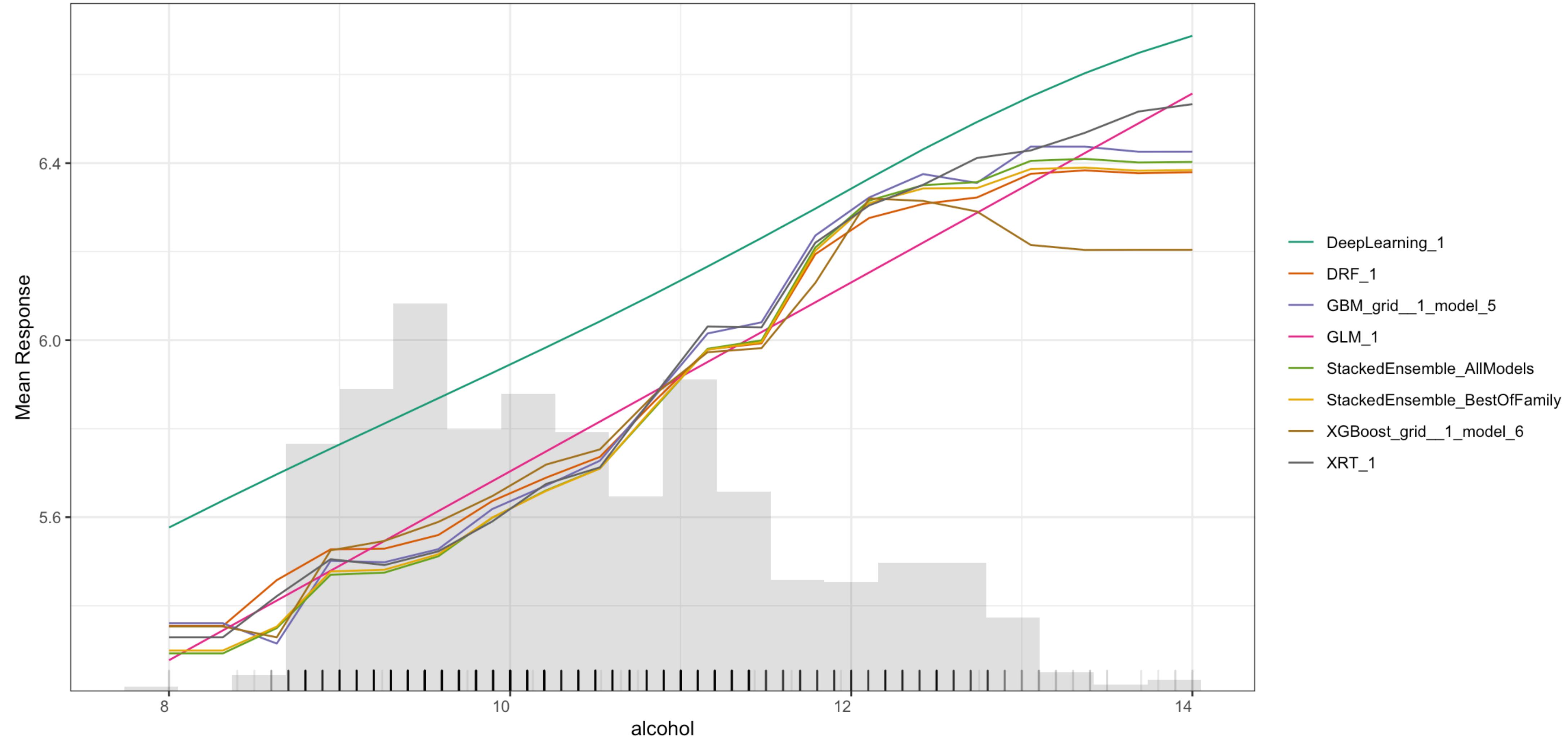


# SHAP Summary

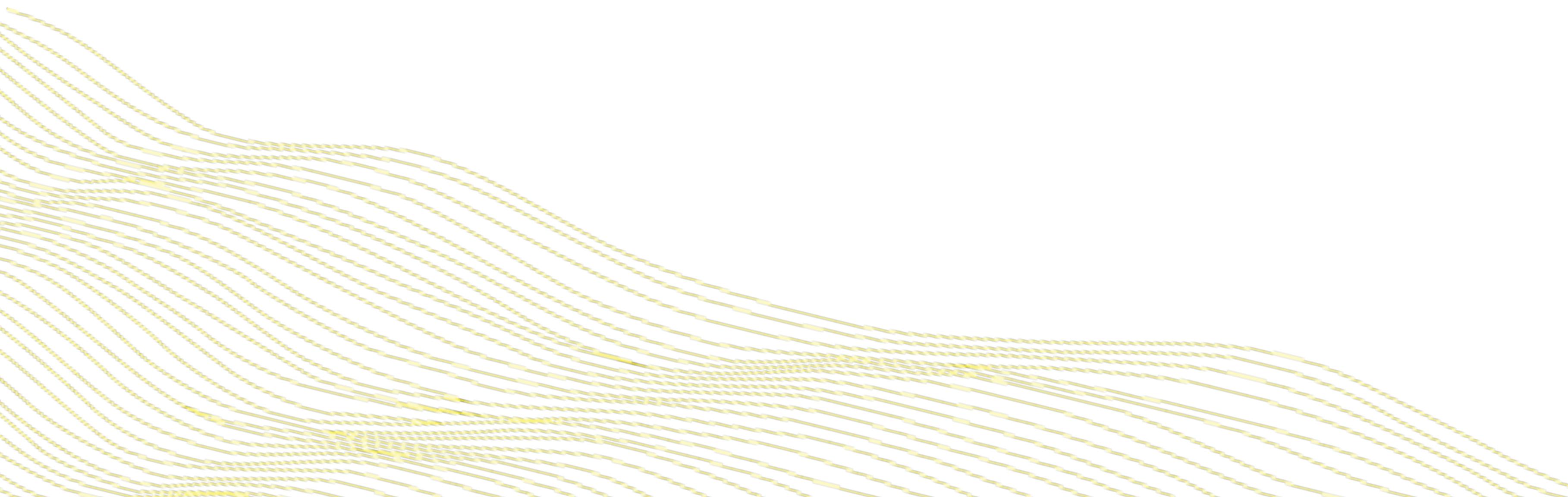


# Partial Dependence (PD) Plots

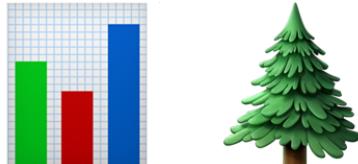
## Partial Dependence on "alcohol"



# Interpretability & Fairness



# Interpretable ML

-  In Machine Learning, "interpretable" refers to techniques and models which are understandable by humans.
-  Some models are inherently interpretable, such as Linear Models or Decision Trees.
-  Note that this is not the same as "Explainable ML" which refers to techniques for helping to explain models (typically black-box models which are not interpretable).

# Fairness in ML

What is "fairness" in ML? 

- Very hard question to answer. 
- Describes a broad set of problems, not a specific approach or metric.

Why it's hard:

- Individual fairness vs. group fairness
- Law/policy is somewhat fuzzy – moving target...

# Fairness in ML

-  Fairness in ML refers to techniques for measuring and/or mitigating the disparate impact on subsets of people defined by "protected" attributes such as age, gender, race, etc.
-  Note that the terms "disparate impact", "adverse impact" and "protected classes" both have colloquial and legal interpretations (and legal doctrine differs by country).

# Protected Attributes for Lending in U.S.

## What is credit discrimination?

The Equal Credit Opportunity Act makes it illegal for a creditor to discriminate in any aspect of credit transaction based on certain characteristics.

In addition, the Fair Housing Act makes many discrimination practices in home financing illegal.

### It is illegal to:

- Refuse you credit if you qualify for it
- Discourage you from applying for credit
- Offer you credit on terms that are less favorable, like a higher interest rate, than terms offered to someone with similar qualifications
- Close your account

### On the basis of:

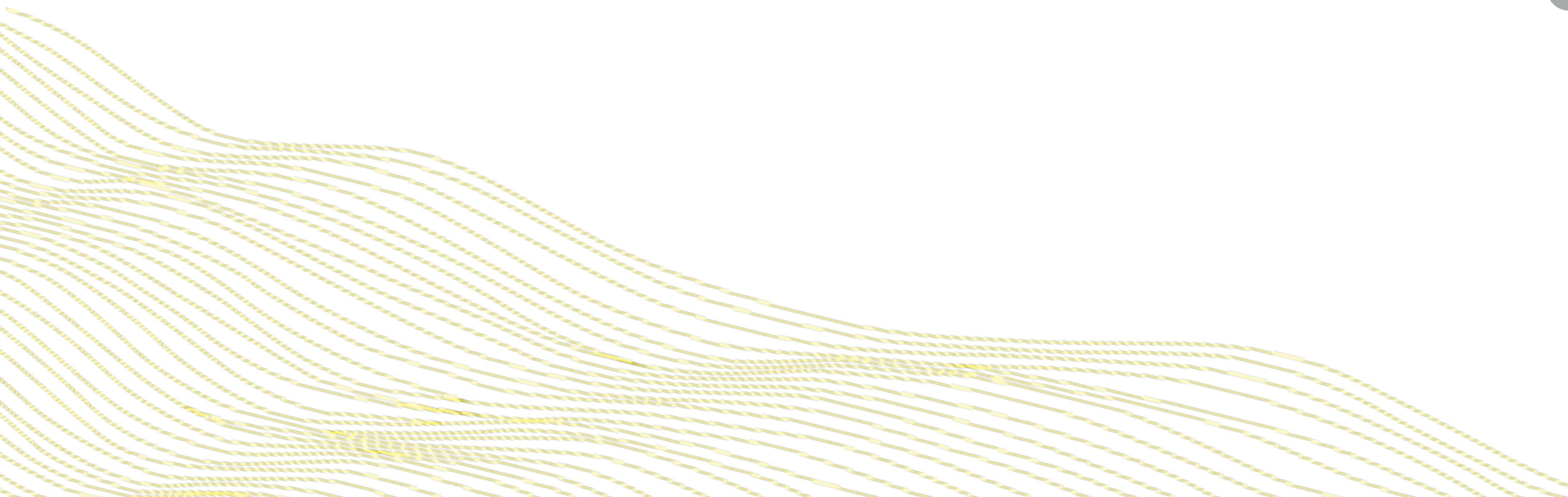
- Race
- Color
- Religion
- National origin
- Sex (including sexual orientation and gender identity)
- Marital status
- Age
- Receiving money from public assistance
- Exercising in good faith your rights under the Consumer Credit Protection Act.



Consumer Financial  
Protection Bureau

-  **Several U.S. laws protect consumers from credit discrimination.**
-  **Lenders must not discriminate based on these attributes.**

# Admissible Machine Learning



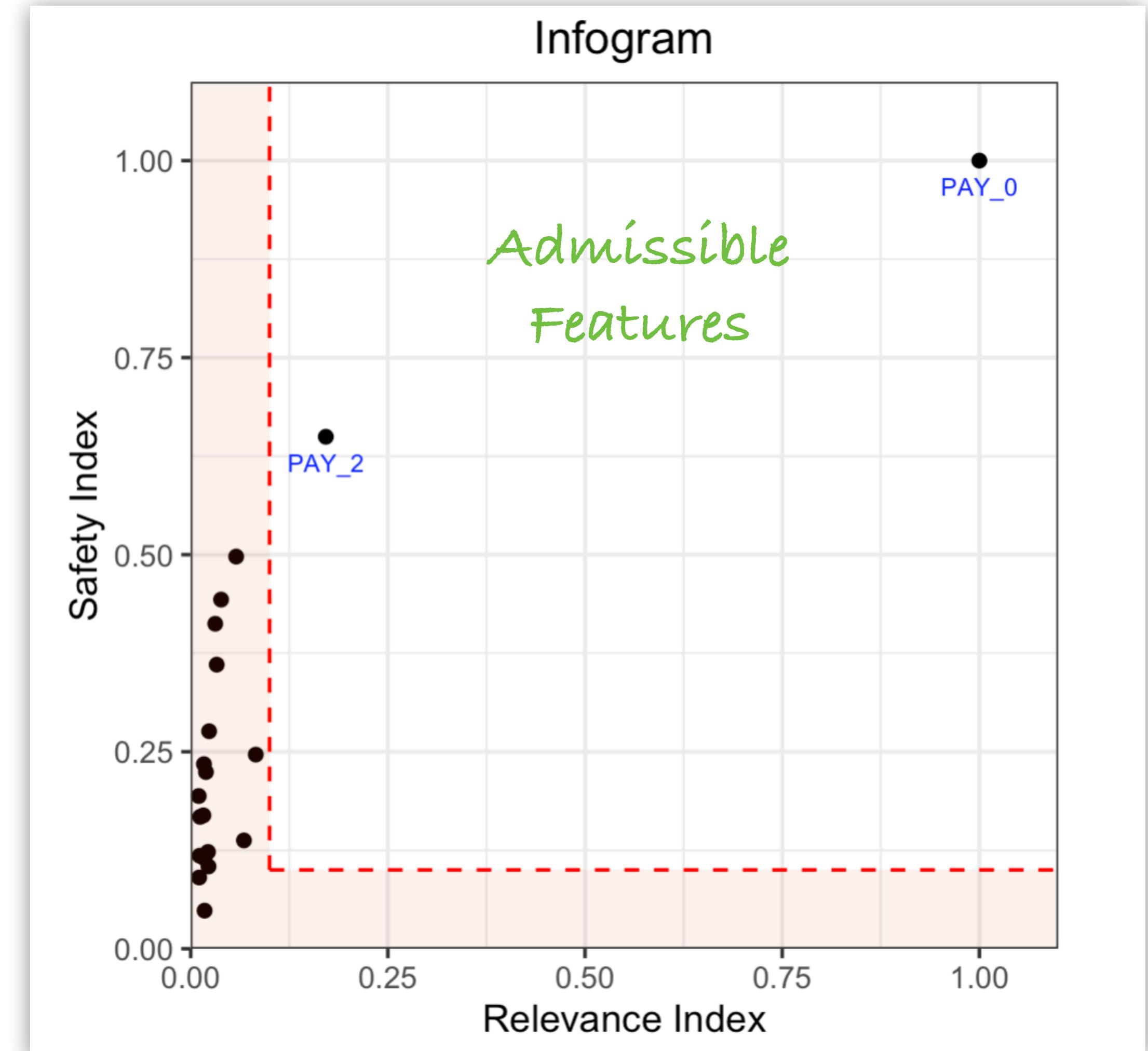
# Goals and Features of Admissible ML

- 🙄 🤫 🤫 Addresses the issue of "Fairness through unawareness" (even if you remove protected variables, you could still have bias in your model).
- 😷 Filter out redundant and/or unsafe variables from your data prior to training models.
- 👩‍⼯ Tackle bias head-on vs. trying to debias models in a post-processing step or via exhaustive search.
- 💫 Easy to use; reduce barriers to safer ML.

# Fair Infogram

⚠ Identify unprotected variables that have high relevance and safety.

- The x-axis is relevance index, a measure of how much the variable drives the response (the more predictive, the higher the relevance).
- The y-axis is safety index, a measure measure of how much extra information the variable has that is not acquired through the protected variables.

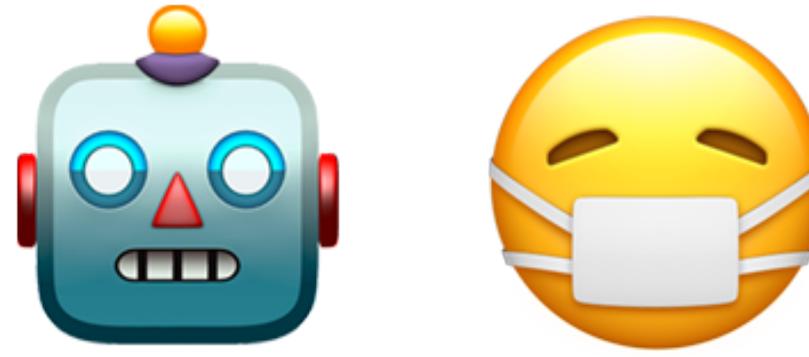


# Admissible AutoML

🤖 In the AutoML context, the goal is usually to maximize model performance 📈 within a fixed budget. 💰

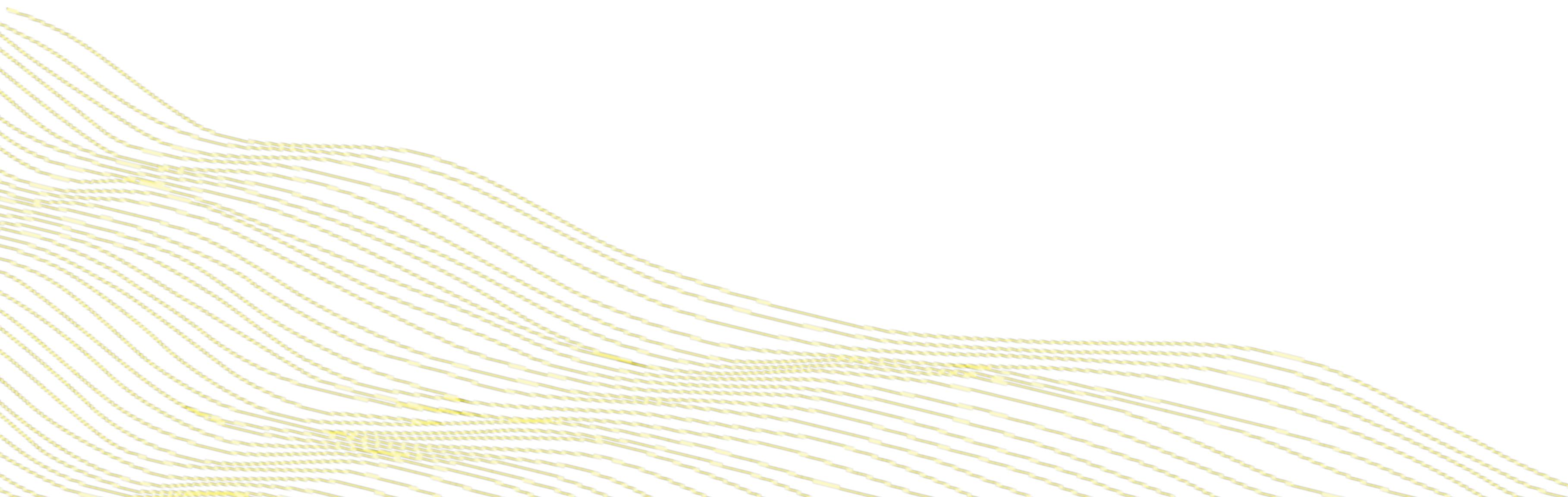
✂️ The reduced, admissible feature set allows us to train models faster and cover a larger search space for the same cost in AutoML systems.

Admissible AutoML is an automatic algorithmic risk-assessment method



⟳ Automatically train models which reduce bias from protected variables by filtering out the inadmissible features.

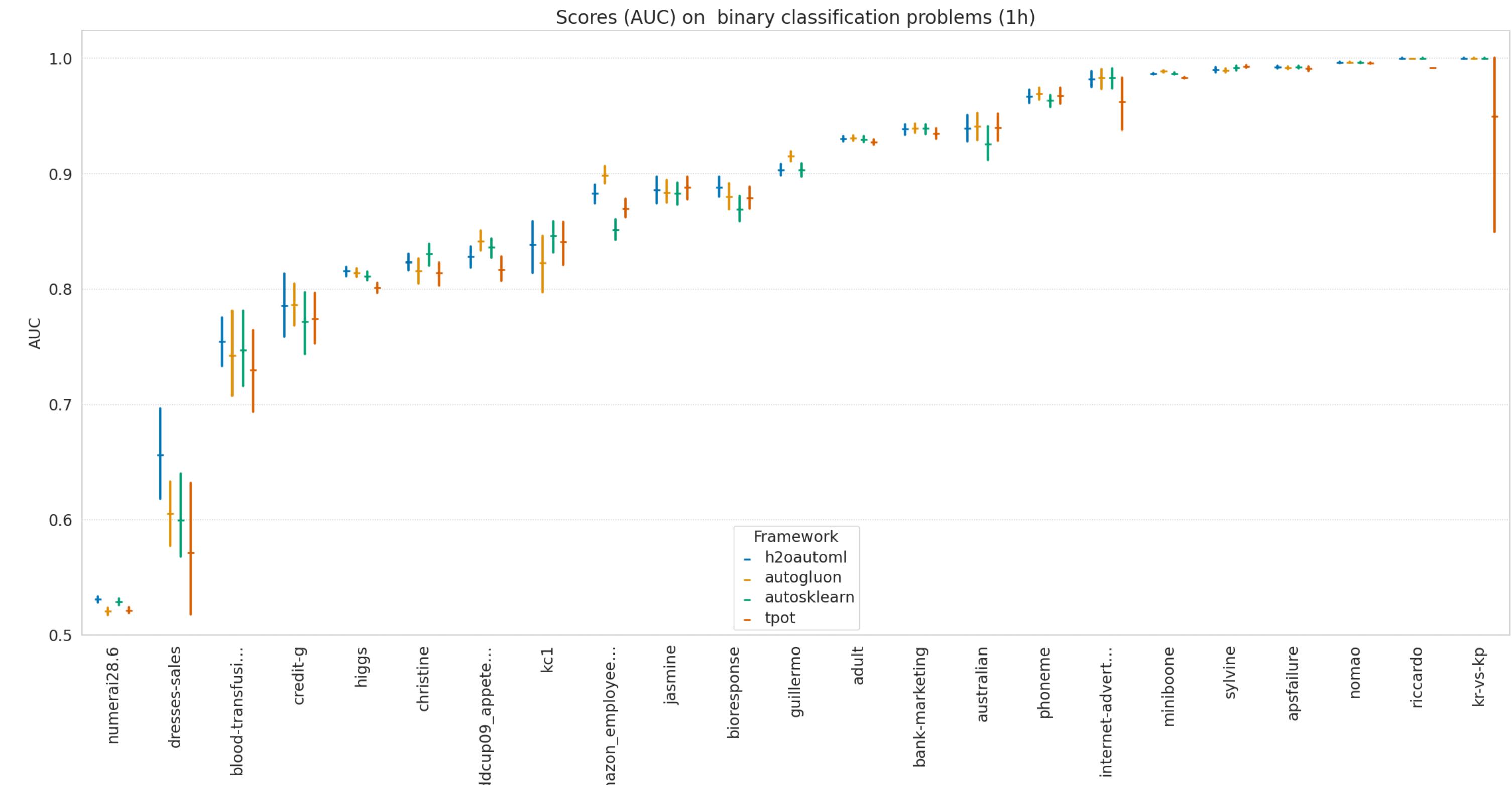
# Resources



# H2O AutoML paper

The H2O AutoML  
paper was published at  
ICML 2020 AutoML  
Workshop

- Official H2O AutoML paper
- Updated benchmarks
- Scalability study (100M rows)
- Stacking study



# Learn H2O!



- Admissible ML Docs: <https://tinyurl.com/h2o-admissible>
- AutoML Docs: <https://tinyurl.com/h2o-automl-docs>
- AutoML tutorials: <https://tinyurl.com/h2o-automl-tutorials>
- Explainability: <https://tinyurl.com/h2o-explain>

# 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>



# Thank you!

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