Towards Scalable Automatic Machine Learning

June 2017

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H2O.ai

Introduction

- Statistician & Machine Learning Scientist at H2O.ai, in Mountain View, California, USA
- Ph.D. in Biostatistics with Designated Emphasis in Computational Science and Engineering from UC Berkeley (focus on Machine Learning)
- Worked as a data scientist at several startups

H2O.ai

H2O.ai

H2O.ai, the Company

- Founded in 2012
- Stanford & Purdue Math & Systems Engineers
- Headquarters: Mountain View, California, USA

H2O, the Platform

- Open Source Software (Apache 2.0 Licensed)
- R, Python, Scala, Java and Web Interfaces
- Distributed Algorithms that Scale to Big Data

Scientific Advisory Council

Dr. Trevor Hastie

- John A. Overdeck Professor of Mathematics, Stanford University
- PhD in Statistics, Stanford University
- Co-author, *The Elements of Statistical Learning: Prediction, Inference and Data Mining*
- Co-author with John Chambers, *Statistical Models in S*
- Co-author, *Generalized Additive Models*

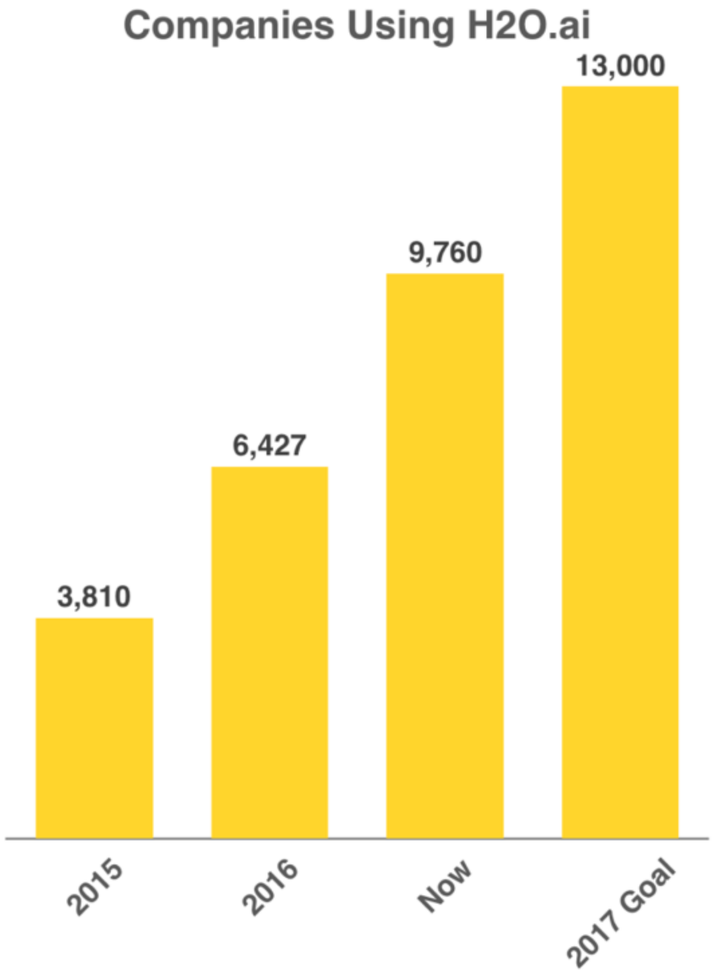
Dr. Robert Tibshirani

- Professor of Statistics and Health Research and Policy, Stanford University
- PhD in Statistics, Stanford University
- 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

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

H2O User Community



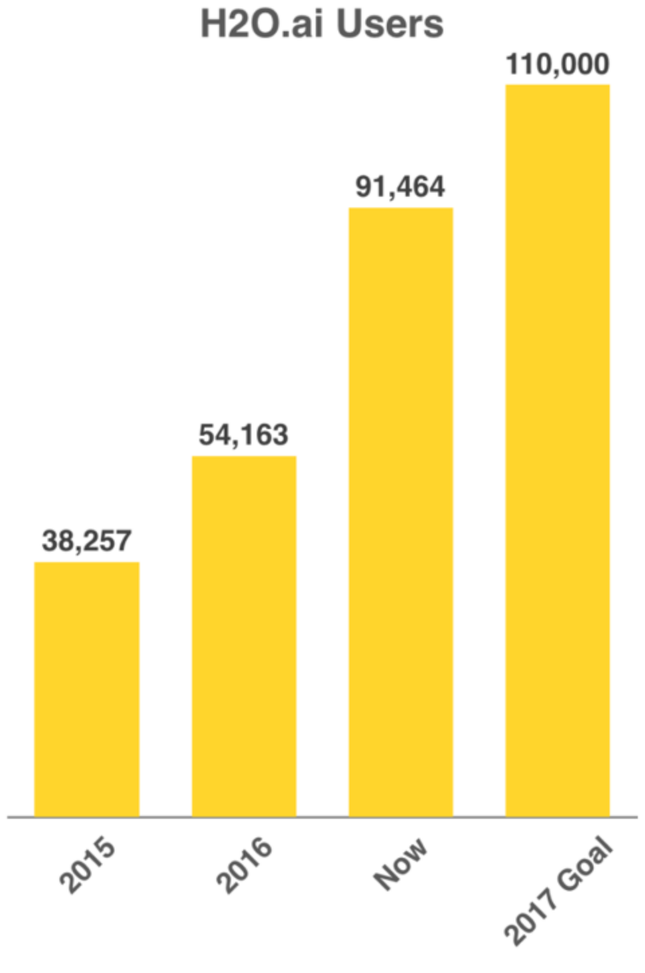
169 OF THE FORTUNE 500

H2O

8 OF TOP 10 BANKS

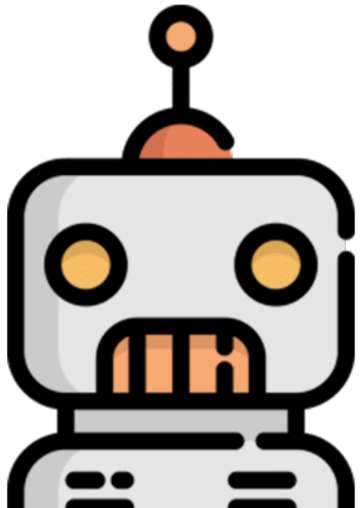
7 OF TOP 10 INSURANCE COMPANIES

4 OF TOP 10 HEALTHCARE COMPANIES

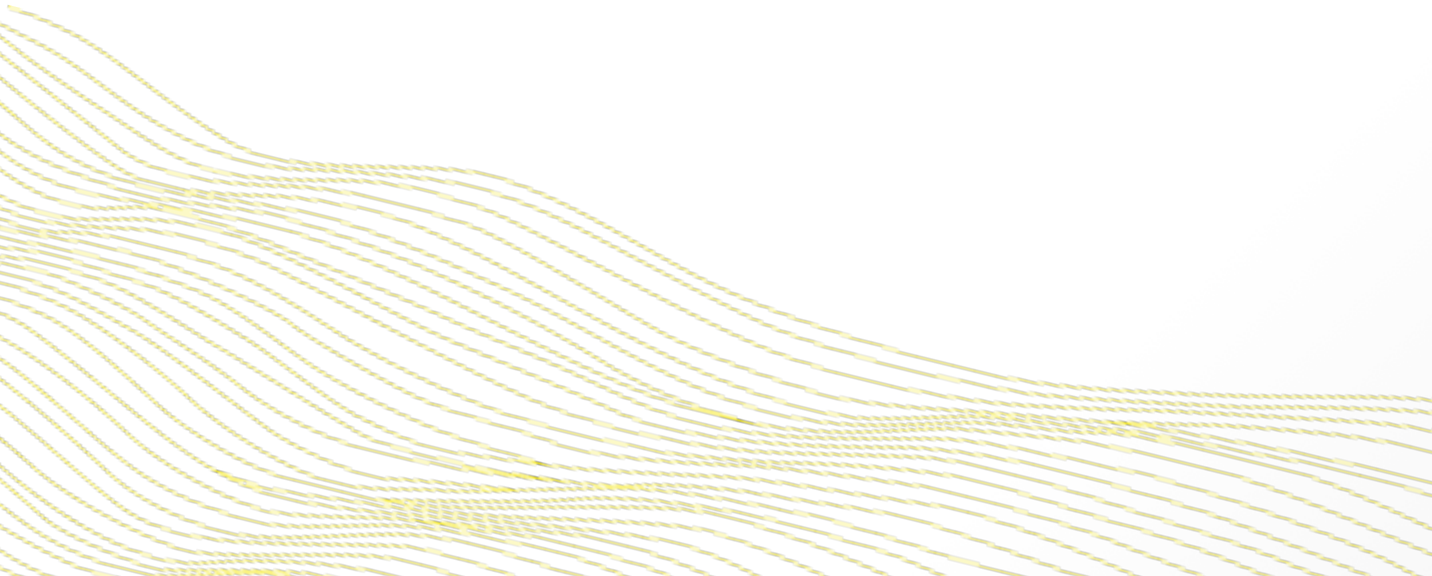


Agenda

- Intro to Automatic Machine Learning (AutoML)
- Bayesian Hyperparamter Optimization
- Random Grid Search
- Stacked Ensembles & Ensemble Selection
- Software for AutoML
- H2O's AutoML



Intro to Automatic Machine Learning



Aspects of Automatic Machine Learning

Data Preprocessing

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

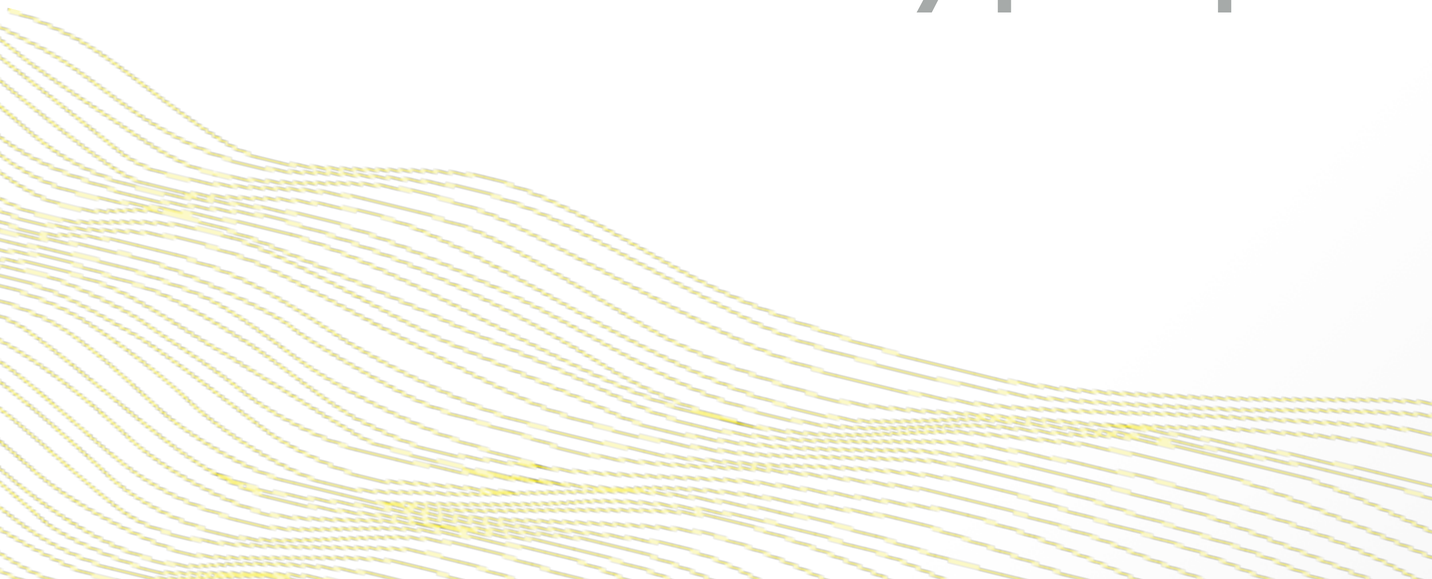
Model Generation

- 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, van der Laan)
- Ensemble Selection (Caruana)

Bayesian Optimization of Hyperparameters



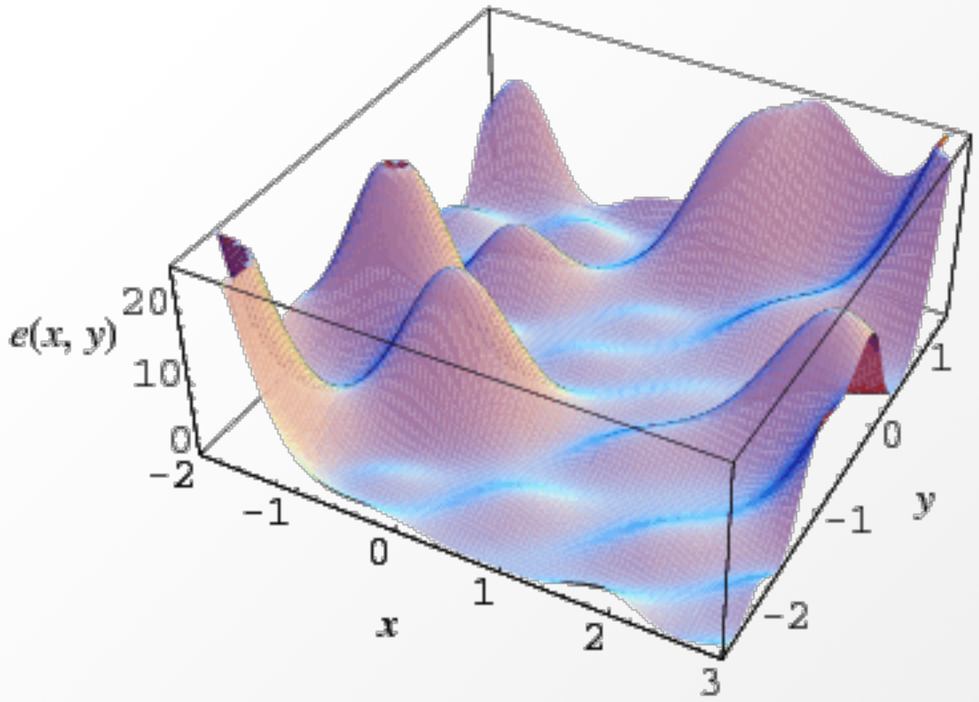
Bayesian Optimization

- Bayesian Hyperparameter Optimization consists of developing a statistical model of the function mapping hyperparameter values to the objective (e.g. AUC, MSE), evaluated on a validation set.
- Different approaches based on: Gaussian Processes, Tree Structured Parzen Estimator, Random Forest

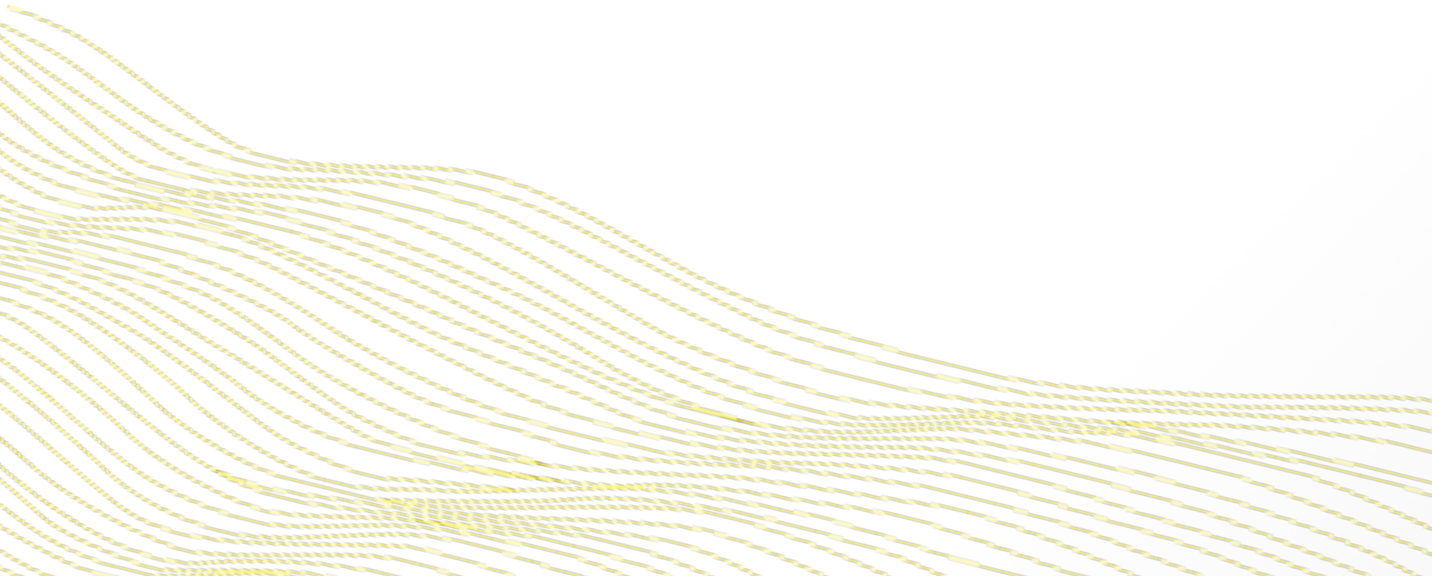
AKA “Sequential Model-based Optimization (SMBO)”

Hyperparameter Optimization Software

- SigOpt (SaaS)
- MOE (C++/Python OSS)
- Scikit-Optimize (Python OSS)
- SMAC (Java OSS)
- Hyperopt (Python OSS)
- Spearmint (Python non-commercial OSS)



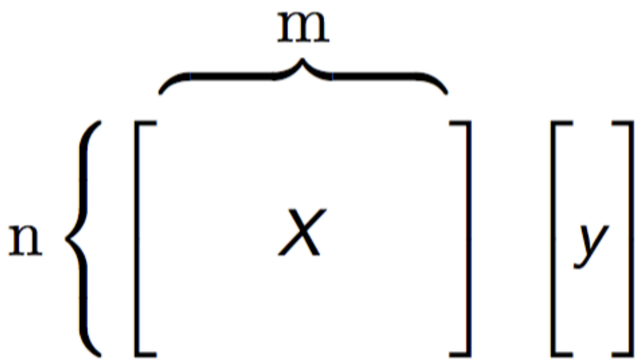
Random Grid Search & Stacked Ensembles



Random Grid Search & Stacking

- In Bengio & Bergstra's 2012 JMLR paper, "Random Search for Hyper-Parameter Optimization", it shows that Random Search is far more efficient than a full (aka Cartesian) Grid Search
- 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

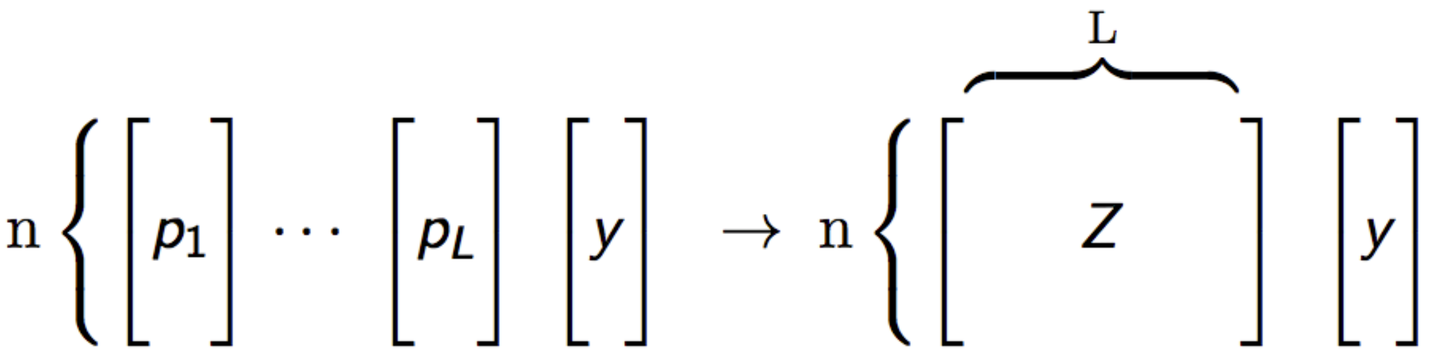
Stacking (aka Super Learner Algorithm)



"Level-zero" data

- Start with design matrix, X, and response, y
- Specify L base learners (with model params)
- Specify a metalearner (just another algorithm)
- Perform k-fold CV on each of the L learners

Stacking (aka Super Learner Algorithm)



"Level-one" data

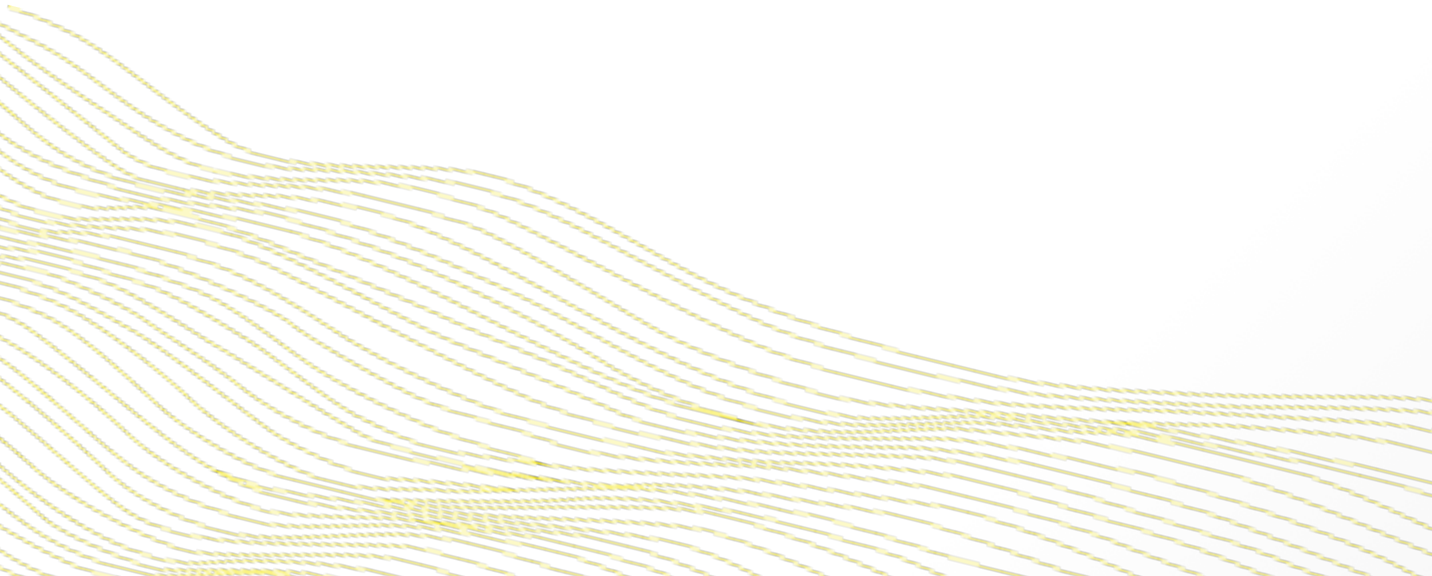
- Collect the predicted values from k-fold CV that was performed on each of the L base learners
- Column-bind these prediction vectors together to form a new design matrix, Z
- Train the metalearner using Z, y

Stacking vs Ensemble Selection

- Stacking uses all the given models (good and bad) and uses a second-level metalearning algorithm to find the optimal combination of base learners.

- With Ensemble Selection, rather than combine good and bad models in an ensemble, forward stepwise selection is used to find a subset of models that, when averaged together, yield the best performance.

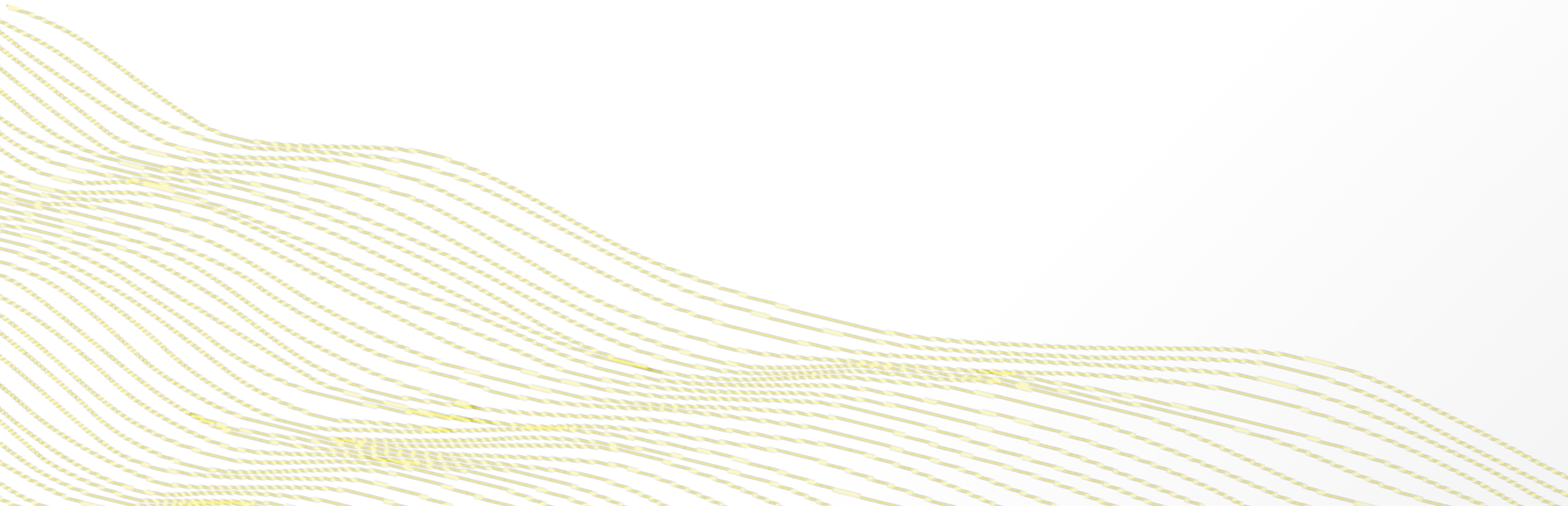
Software for AutoML



Open Source AutoML Software

- H2O AutoML (Java w/ APIs in Python, R, Scala, and a web GUI)
- auto-sklearn (Python)
- AutoWEKA (Java)
- TPOT (Python)
- auto_ml (Python)

H2O AutoML



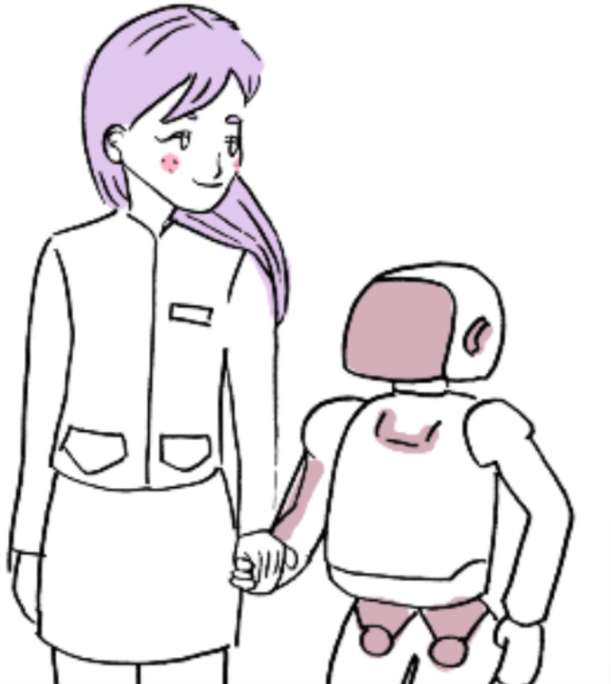
H2O AutoML

- Very simple interface to define the data, response column and stopping strategy.
- Automatic data pre-processing (as in all H2O algos).
- Individual models are tuned using a validation set.
- Also trains random grid of GBMs, DNNs, GLMs, etc. using a carefully chosen parameter space.
- A Stacked Ensemble is trained using all models.
- Returns a sorted "Leaderboard" of all models.

Available in Bleeding Edge release of H2O!

H2O AutoML R & Python Demos

- Documentation, R and Python code examples are available in the H2O User Guide at http://docs.h2o.ai.
- Live demo time!



```
aml <- h2o.automl(x = x, y = y,
                  training_frame = train,
                  leaderboard_frame = test,
                  max_runtime_secs = 30)
```

H2O Resources

- Documentation: http://docs.h2o.ai
- Tutorials: https://github.com/h2oai/h2o-tutorials
- Slidedecks: https://github.com/h2oai/h2o-meetups
- Video Presentations: https://www.youtube.com/user/0xdata
- Events & Meetups: http://h2o.ai/events

Thank you!

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http://www.stat.berkeley.edu/~ledell