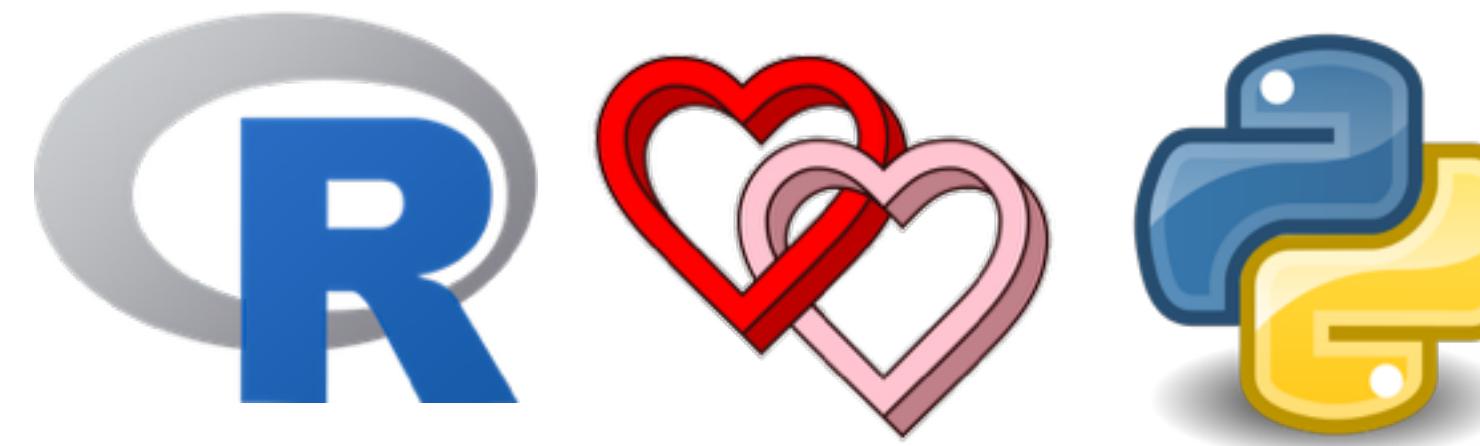


Scalable Machine Learning in R and Python with H2O



R-Ladies & PyLadies Meetup

Barcelona, Spain Dec 2016

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Machine Learning Scientist
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
- Co-organizer of R-Ladies San Francisco and co-founder of R-Ladies Global (rladies.org)
- Founder of “Women in Machine Learning & Data Science” (wimlds.org) Meetup organization



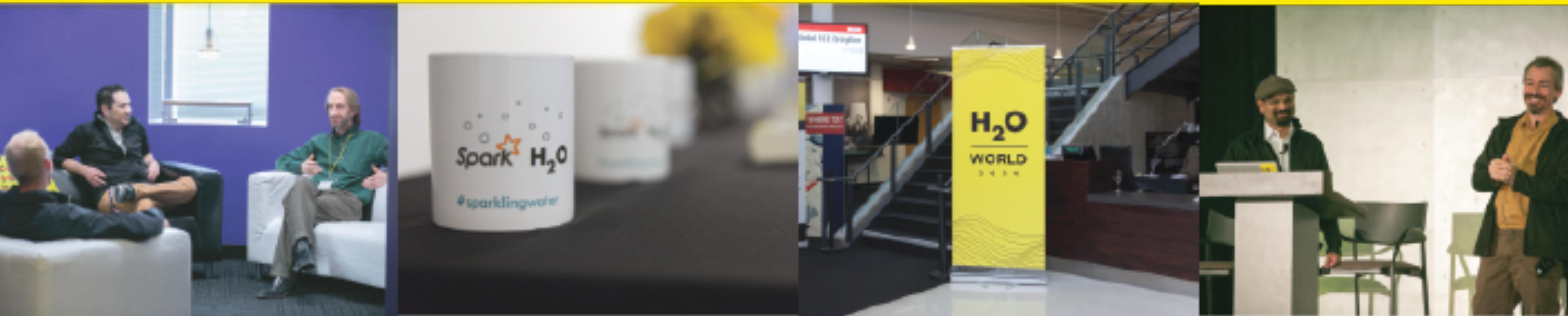
Agenda



- Who/What is H2O?
- Machine Learning 101
- H2O Machine Learning Platform
- H2O in R & Python
- Tutorials: Intro, Grid, DL, Stacking
- New/active developments in H2O



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

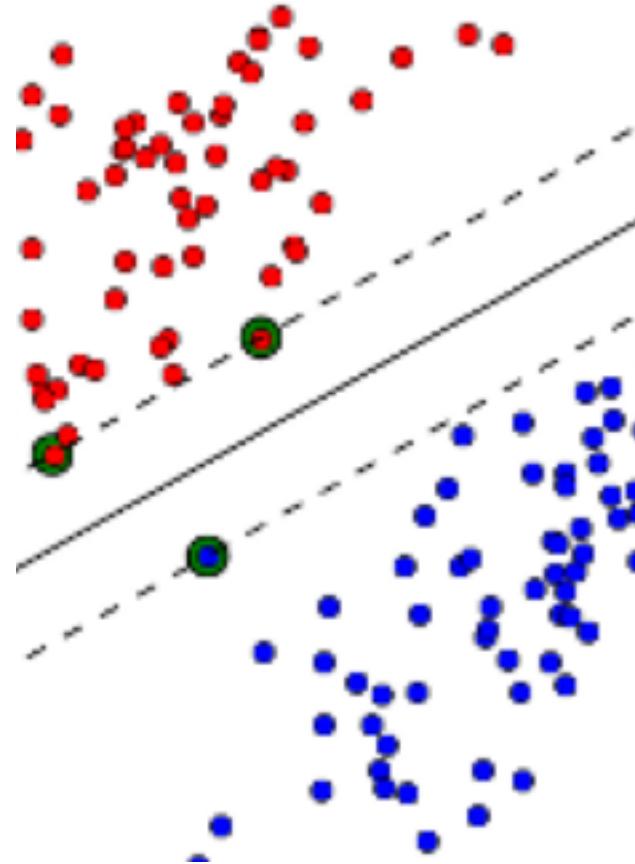
- Professor of Statistics and Health Research and Policy, Stanford University
- PhD in Statistics, Stanford University
- Co-author, *The Elements of Statistical Learning: Prediction, Inference and Data Mining*
- Author, *Regression Shrinkage and Selection via the Lasso*
- Co-author, *An Introduction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

What is Machine Learning?



"Field of study that gives computers the ability to learn without being explicitly programmed."

— Arthur Samuel, 1959

Unlike rules-based systems which require a human expert to hard-code domain knowledge directly into the system, a machine learning algorithm learns how to make decisions from the data alone.

Machine Learning Tasks

Regression

- Predict a real-valued response (e.g. price, weight)
 - Response distribution: Gaussian, Gamma, Poisson, etc.
 - Evaluate with MSE, MAE or R²
-

Classification

- Multi-class or binary classification
 - Ranking (e.g. Google Search results order)
 - Evaluate with Classification Error or AUC
-

Clustering

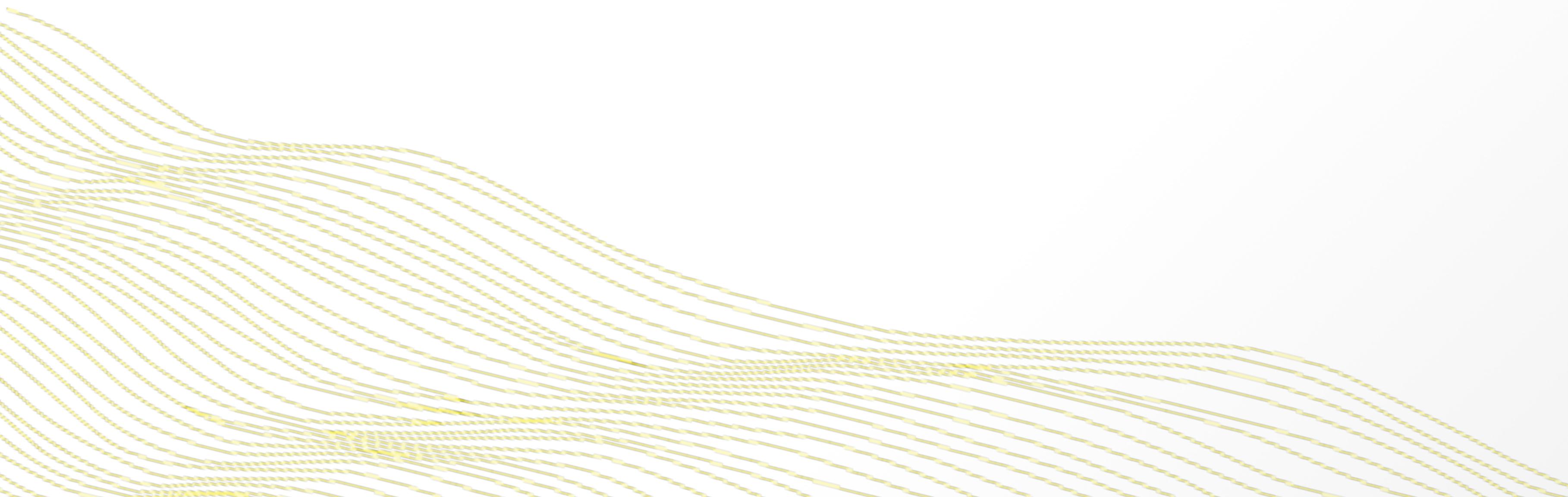
- Unsupervised learning (no training labels)
- Partition the data; identify clusters or sub-populations
- Evaluate with AIC, BIC or Total Sum of Squares

Train, Validation and Test Set



- If you plan on doing any model tuning, you should split your dataset into three parts: Train, Validation and Test
- There is no general rule for how you should partition the data and it will depend on how strong the signal in your data is, but an example could be:
50% Train, 25% Validation and 25% Test
- The validation set is used strictly for model tuning and the test set is used to make a final estimate of the generalization error.

H2O Platform



H2O Platform Overview

- Distributed implementations of cutting edge ML algorithms.
- Core algorithms written in high performance Java.
- APIs available in R, Python, Scala, REST/JSON.
- Interactive Web GUI called H2O Flow.
- Easily deploy models to production with H2O Steam.



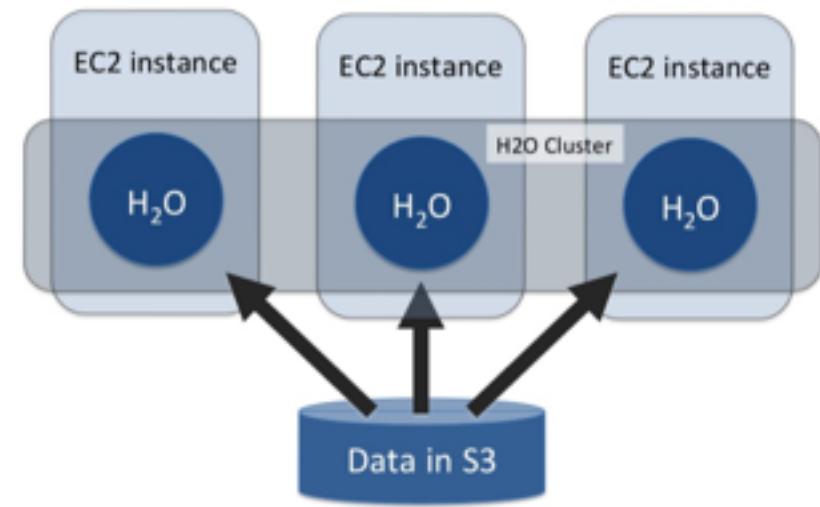
H2O Platform Overview

- Write code in high-level language like R (or use the web GUI) and output production-ready models in Java.
- To scale, just add nodes to your H2O cluster.
- Works with Hadoop, Spark and your laptop.



H2O Distributed Computing

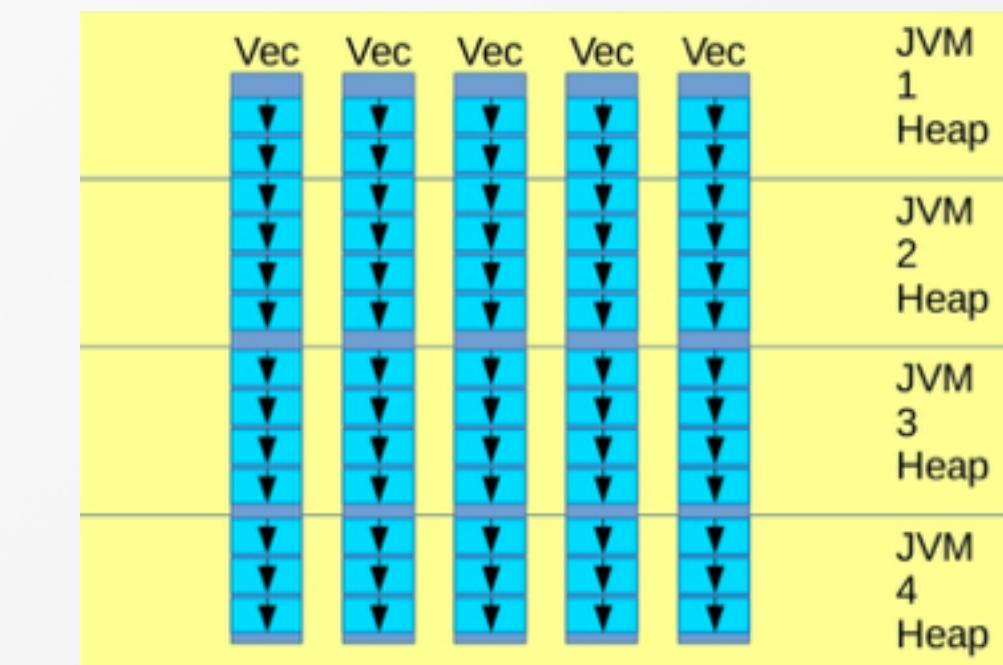
H2O Cluster



- Multi-node cluster with shared memory model.
- All computations in memory.
- Each node sees only some rows of the data.
- No limit on cluster size.

H2O Frame

- Distributed data frames (collection of vectors).
- Columns are distributed (across nodes) arrays.
- Works just like R's `data.frame` or Python Pandas `DataFrame`



Current Algorithm Overview

Statistical Analysis

- Linear Models (GLM)
- Naïve Bayes

Ensembles

- Random Forest
- Distributed Trees
- Gradient Boosting Machine
- R Package - Stacking / Super Learner

Deep Neural Networks

- Multi-layer Feed-Forward Neural Network
- Auto-encoder
- Anomaly Detection
- Deep Features

Clustering

- K-Means

Dimension Reduction

- Principal Component Analysis
- Generalized Low Rank Models

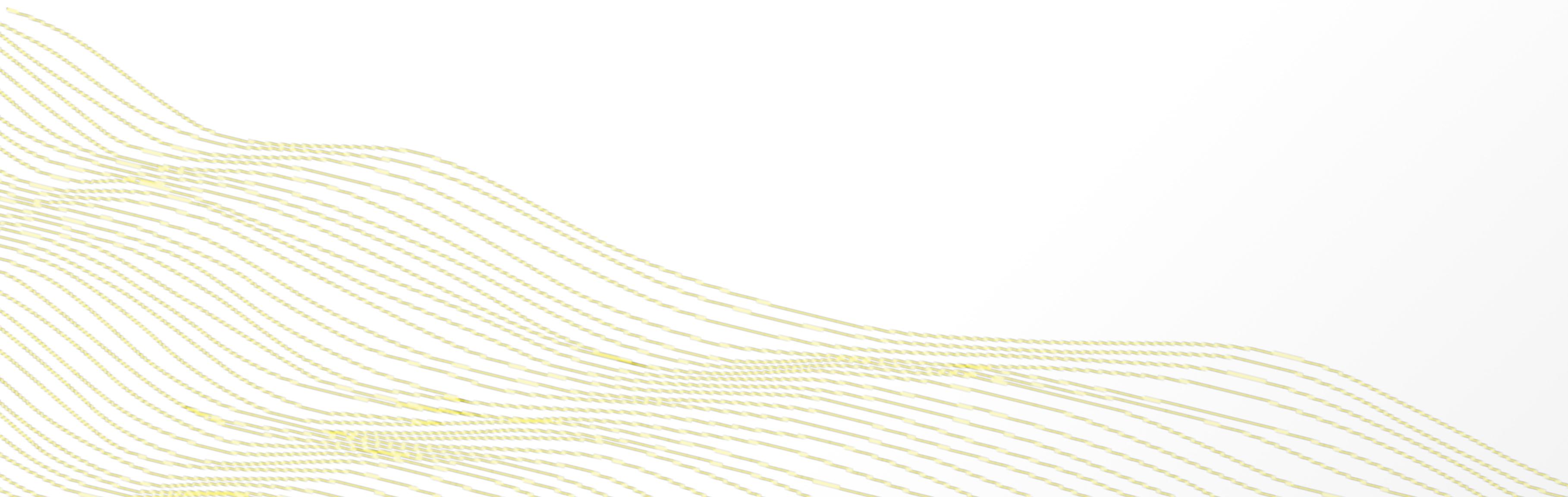
Solvers & Optimization

- Generalized ADMM Solver
- L-BFGS (Quasi Newton Method)
- Ordinary Least-Square Solver
- Stochastic Gradient Descent

Data Munging

- Scalable Data Frames
- Sort, Slice, Log Transform

H₂O in R



h2o R Package



Installation

- Java 7 or later; R 3.1 and above; Linux, Mac, Windows
- The easiest way to install the h2o R package is CRAN.
- Latest version: <http://www.h2o.ai/download/h2o/r>

Design

All computations are performed in highly optimized Java code in the H2O cluster, initiated by REST calls from R.

h2o Python Module



Installation

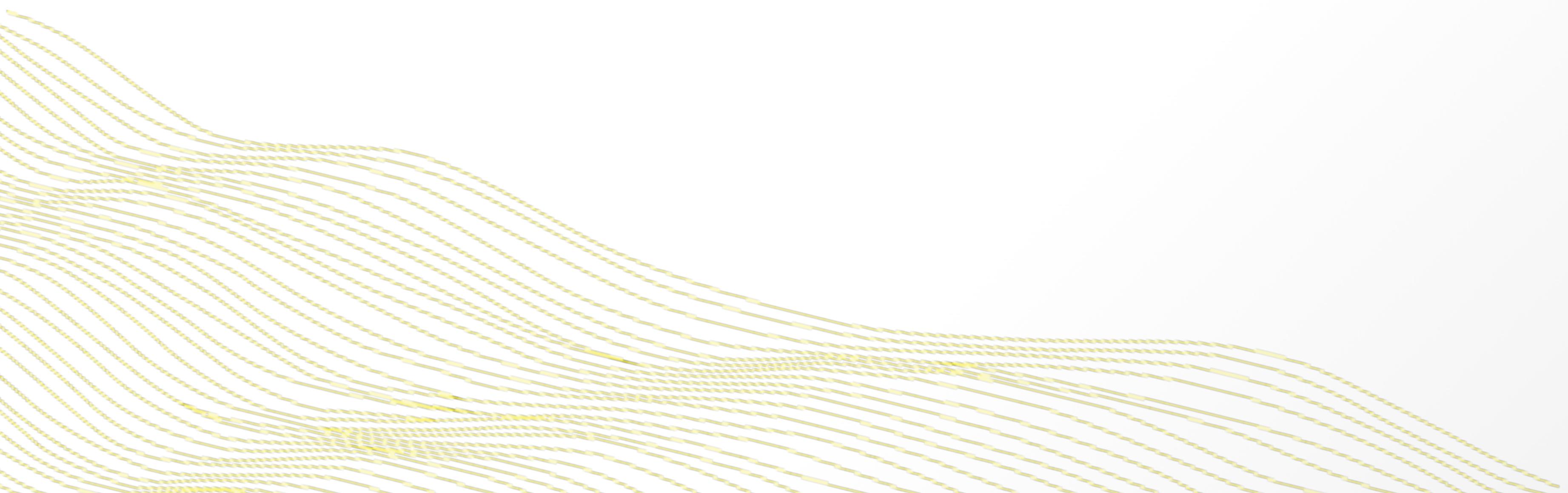
- Java 7 or later; Python 2.7, 3.5; Linux, Mac, Windows
- The easiest way to install the h2o Python module is PyPi.
- Latest version: <http://www.h2o.ai/download/h2o/python>

Design

All computations are performed in highly optimized Java code in the H2O cluster, initiated by REST calls from Python.

H2O R & Python Tutorials

<https://github.com/h2oai/h2o-tutorials>



R & Py Tutorial: Intro to H2O Algorithms

The “Intro to H2O” tutorial introduces five popular supervised machine learning algorithms in the context of a binary classification problem.

The training module demonstrates how to train models and evaluate model performance on a test set.

- Generalized Linear Model (GLM)
- Random Forest (RF)
- Gradient Boosting Machine (GBM)
- Deep Learning (DL)
- Naive Bayes (NB)

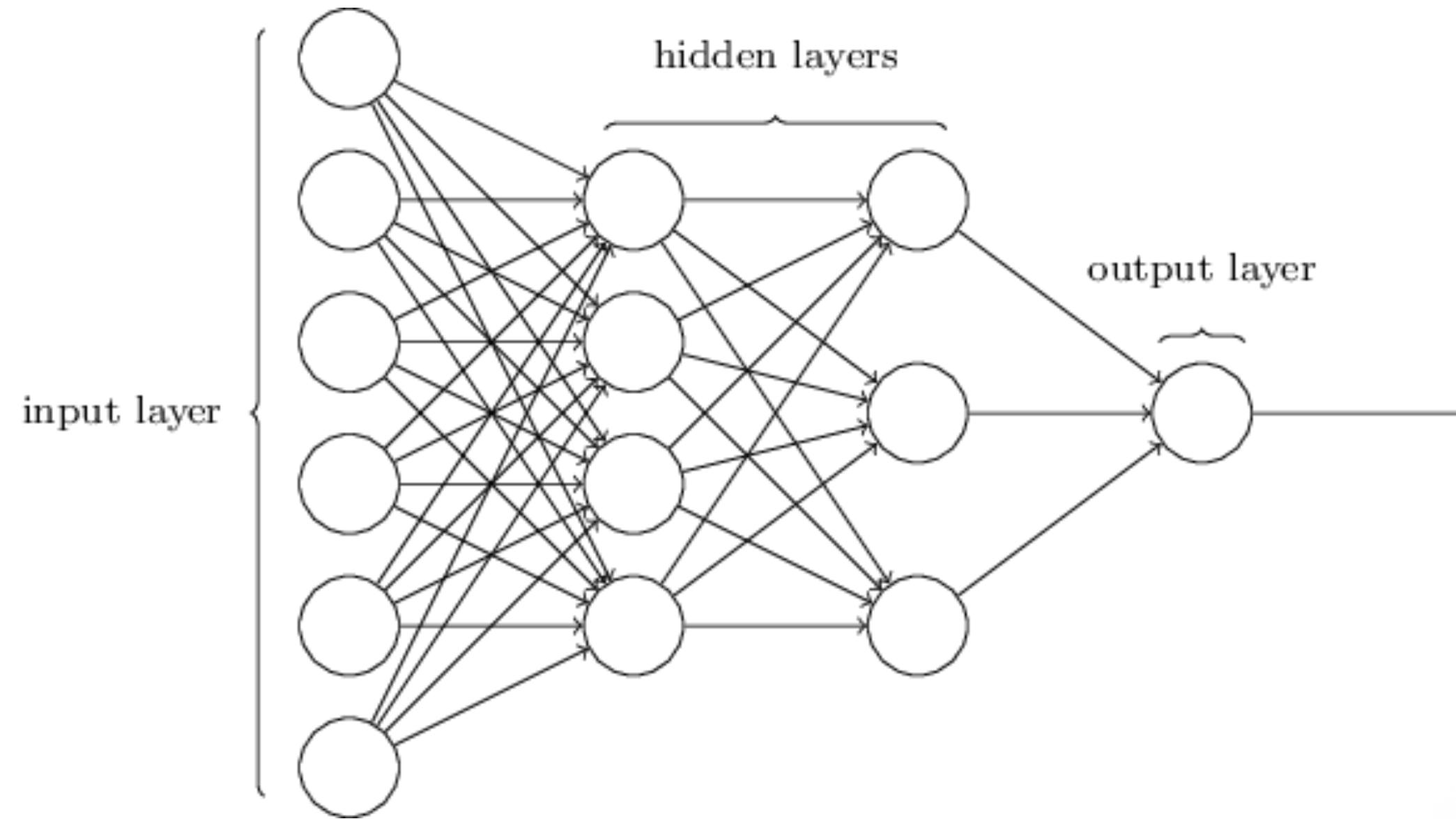
R & Py Tutorial: Grid Search for Model Selection

```
> print(gbm_gridperf)
H2O Grid Details
=====
Grid ID: gbm_grid2
Used hyper parameters:
- sample_rate
- max_depth
- learn_rate
- col_sample_rate
Number of models: 72
Number of failed models: 0

Hyper-Parameter Search Summary: ordered by decreasing auc
  sample_rate max_depth learn_rate col_sample_rate      model_ids          auc
1           1         3       0.19  1 gbm_grid2_model_38 0.685166598389755
2           0.9       3       0.15  1 gbm_grid2_model_53 0.684956999713052
3           0.8       5       0.06  1 gbm_grid2_model_22 0.684843506375254
4           0.6       4       0.07  1 gbm_grid2_model_4   0.684327718715252
5           0.95      4       0.13  1 gbm_grid2_model_48 0.684042497773235
```

The second training module demonstrates how to find the best set of model parameters for each model using Grid Search.

R Tutorial: Deep Learning



The “Deep Learning in R” tutorial gives an overview of how to train H2O deep neural networks in R.

- Deep Learning via Multilayer Perceptrons (MLPs)
 - Early Stopping
 - Random Grid Search
- Deep Learning Autoencoders
- Unsupervised Pretraining
 - Deep Features
 - Anomaly Detection

R Tutorial: Ensembles via Stacking

```
> perf <- h2o.ensemble_performance(fit, newdata = test)
|-----| 100%
|-----| 100%
|-----| 100%
|-----| 100%
>
> perf

Base learner performance, sorted by specified metric:
  learner      AUC
1   h2o.glm.wrapper 0.6871177
4 h2o.deeplearning.wrapper 0.7172476
2 h2o.randomForest.wrapper 0.7653992
3   h2o.gbm.wrapper 0.7817096

H2O Ensemble Performance on <newdata>:
-----
Family: binomial

Ensemble performance (AUC): 0.785726880397054
>
```



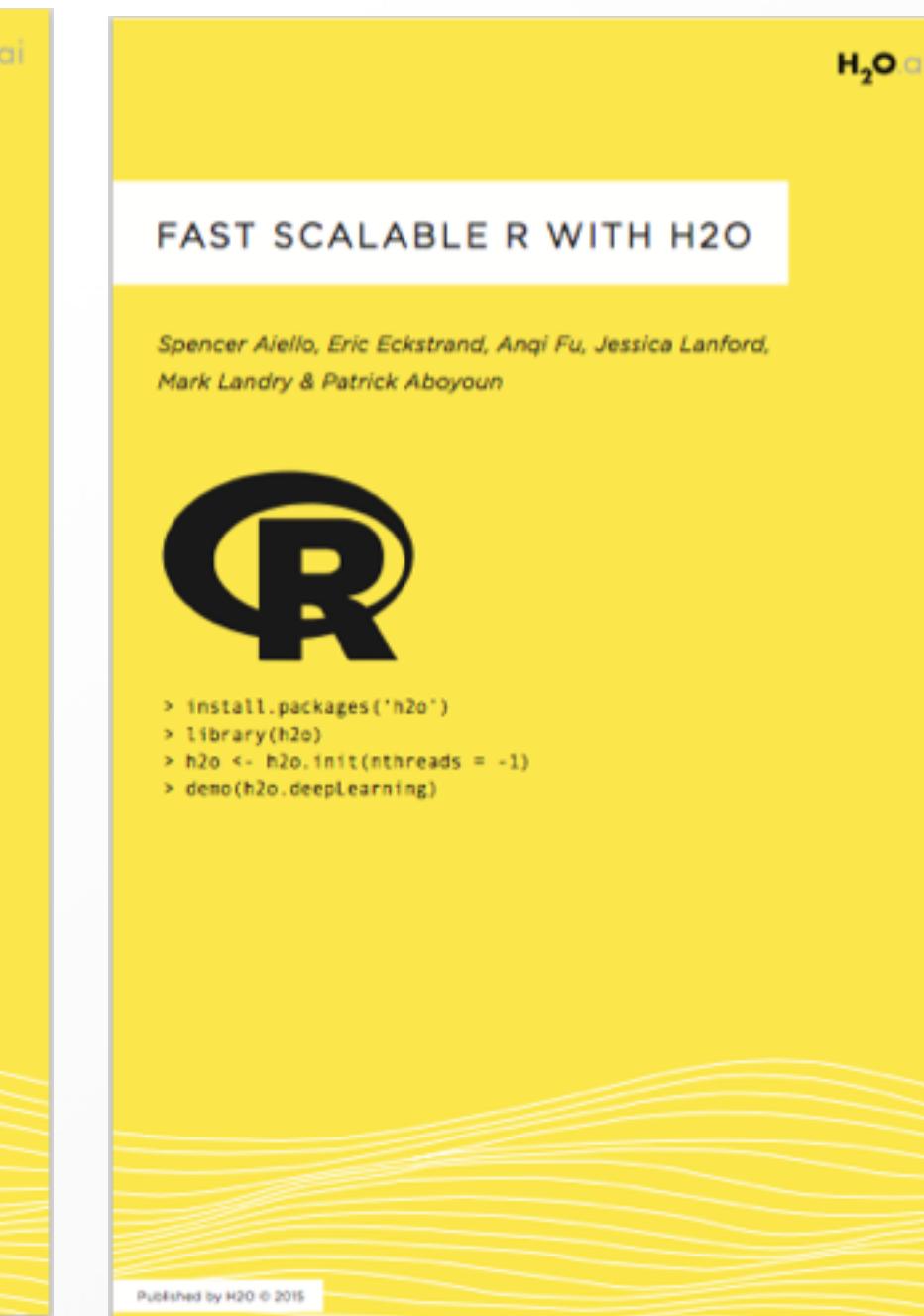
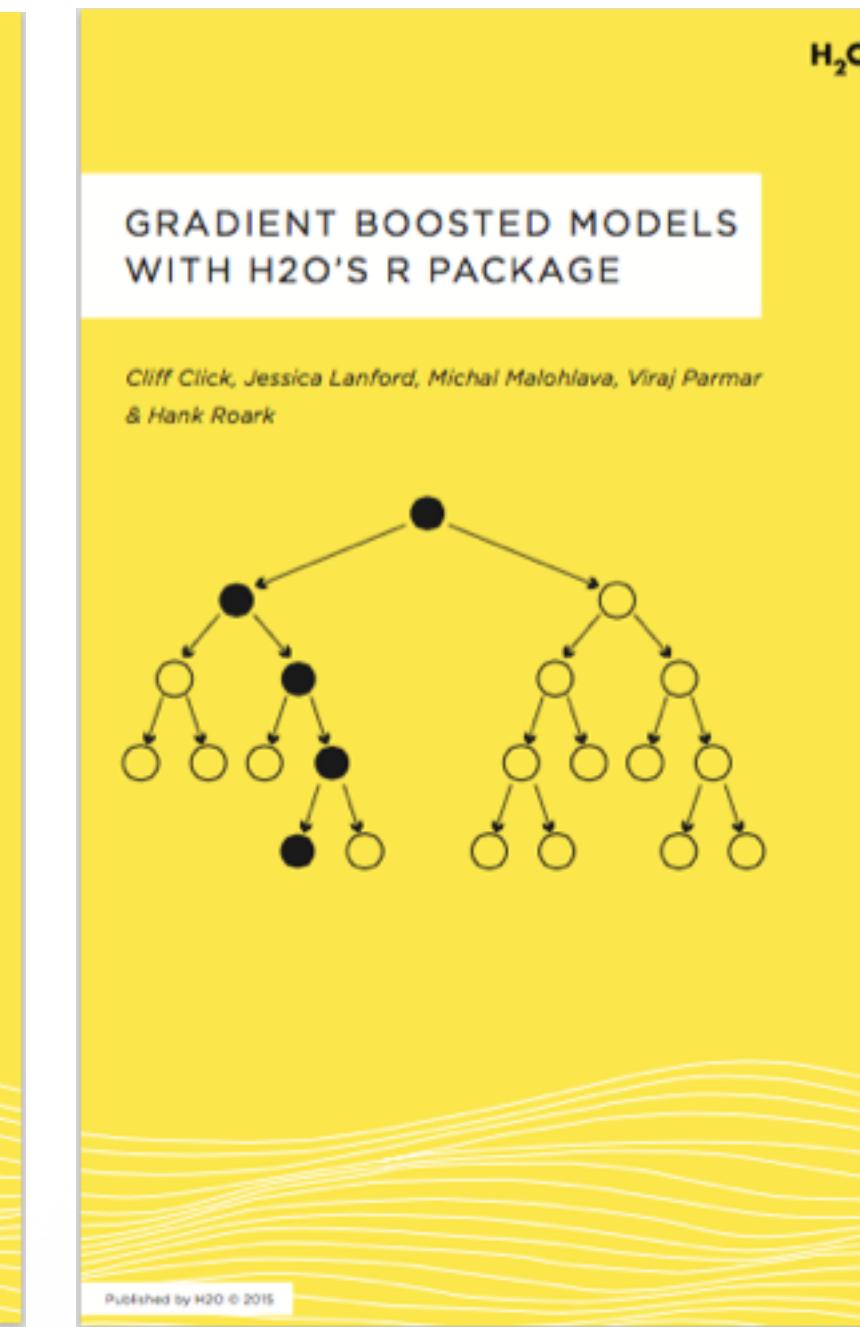
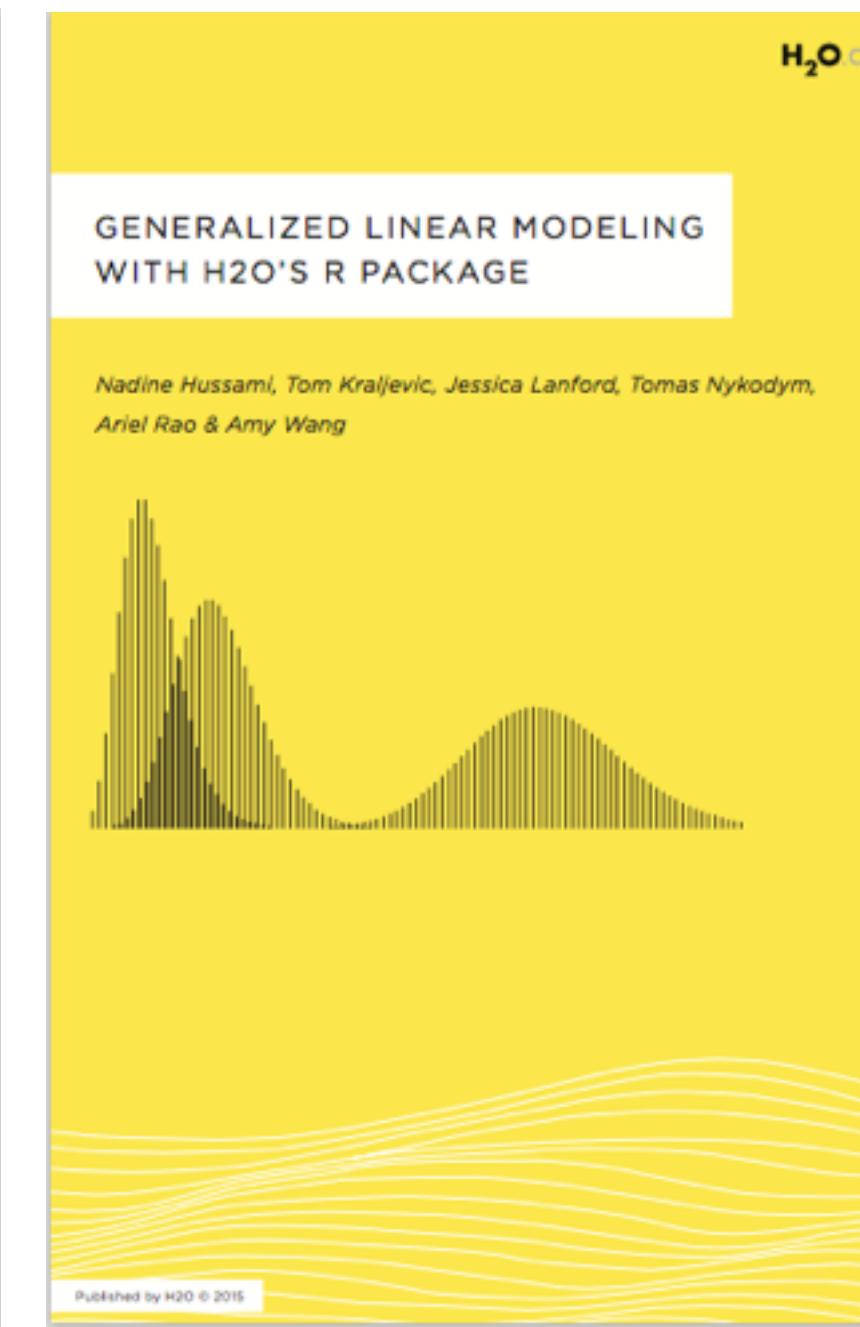
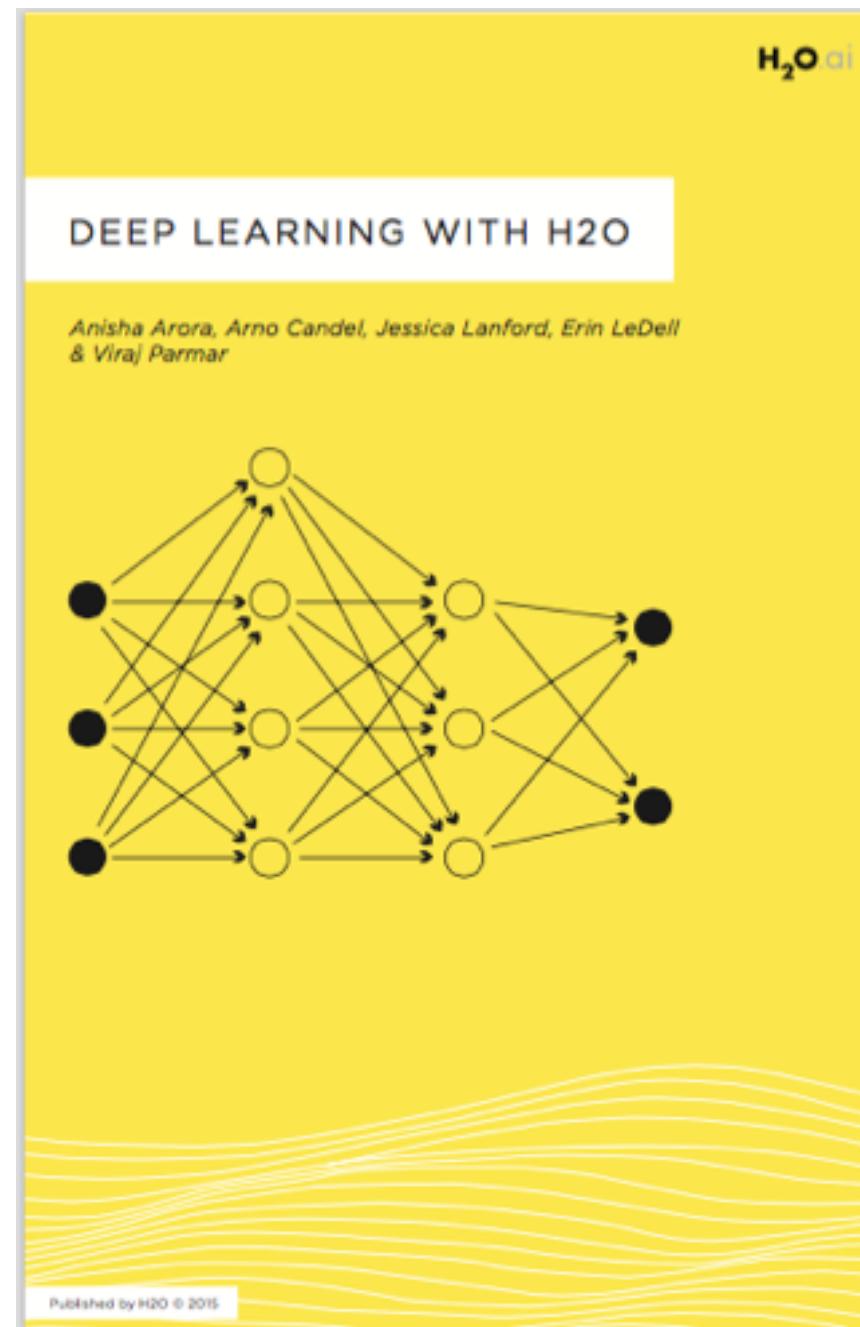
The “H2O Ensemble” Tutorial
demonstrates how to use the `h2oEnsemble`
R package which extends the `h2o` R API.

H2O Resources

- Online Training: <http://learn.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>
- Community: <https://community.h2o.ai>



H2O Booklets



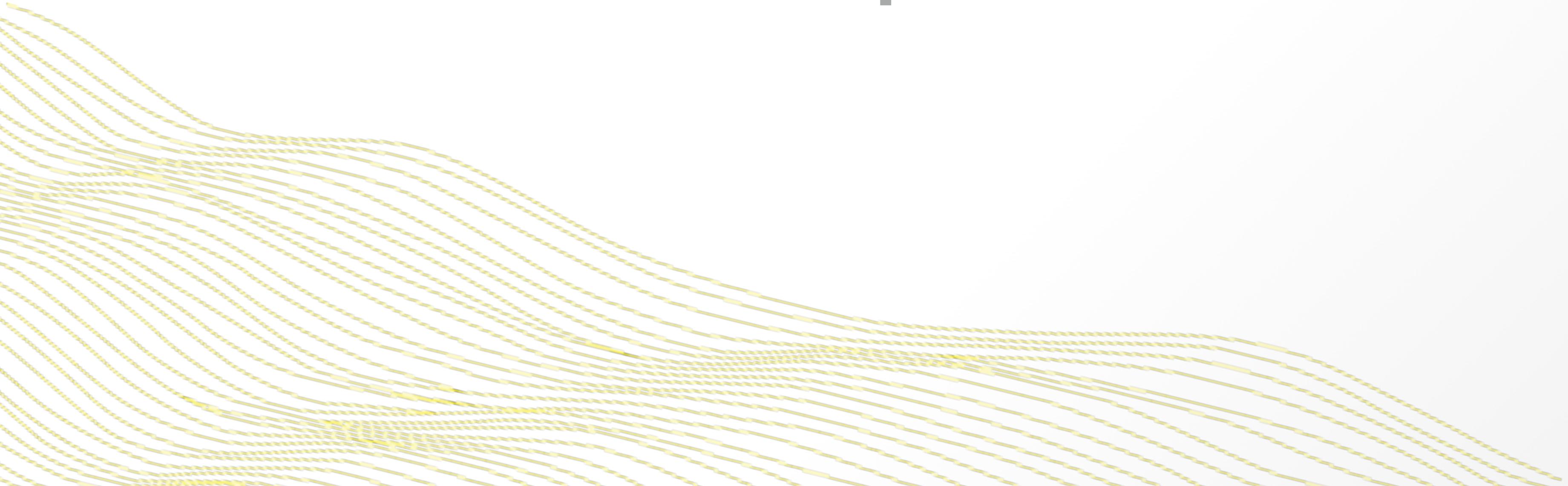
<http://docs.h2o.ai/>

Thank you!

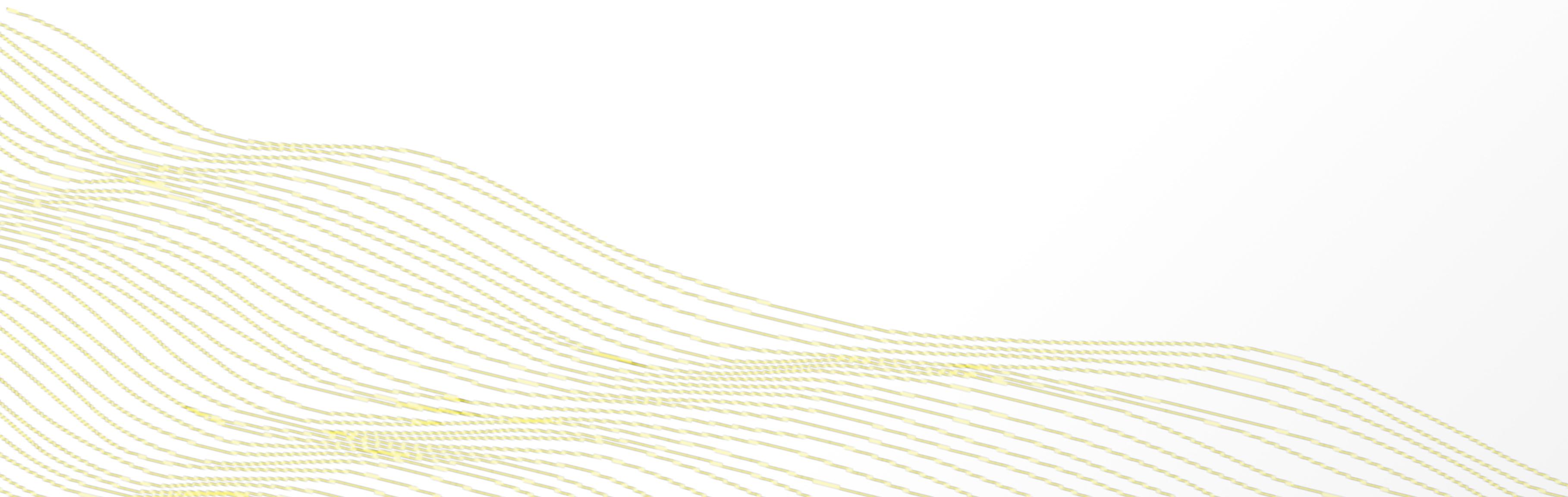
@ledell on Github, Twitter
erin@h2o.ai

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

Appendix: New & Active Developments in H₂O

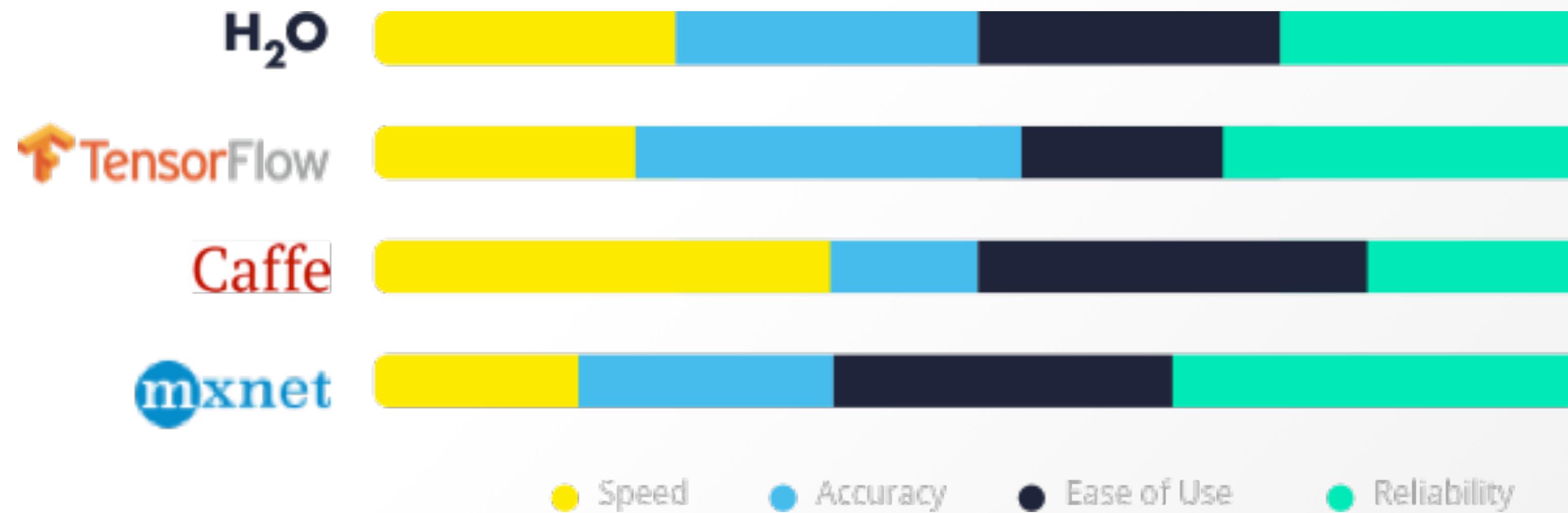


Deep Water



Deep Water

Project “Deep Water” is a unification of the top open source libraries for Deep Learning.

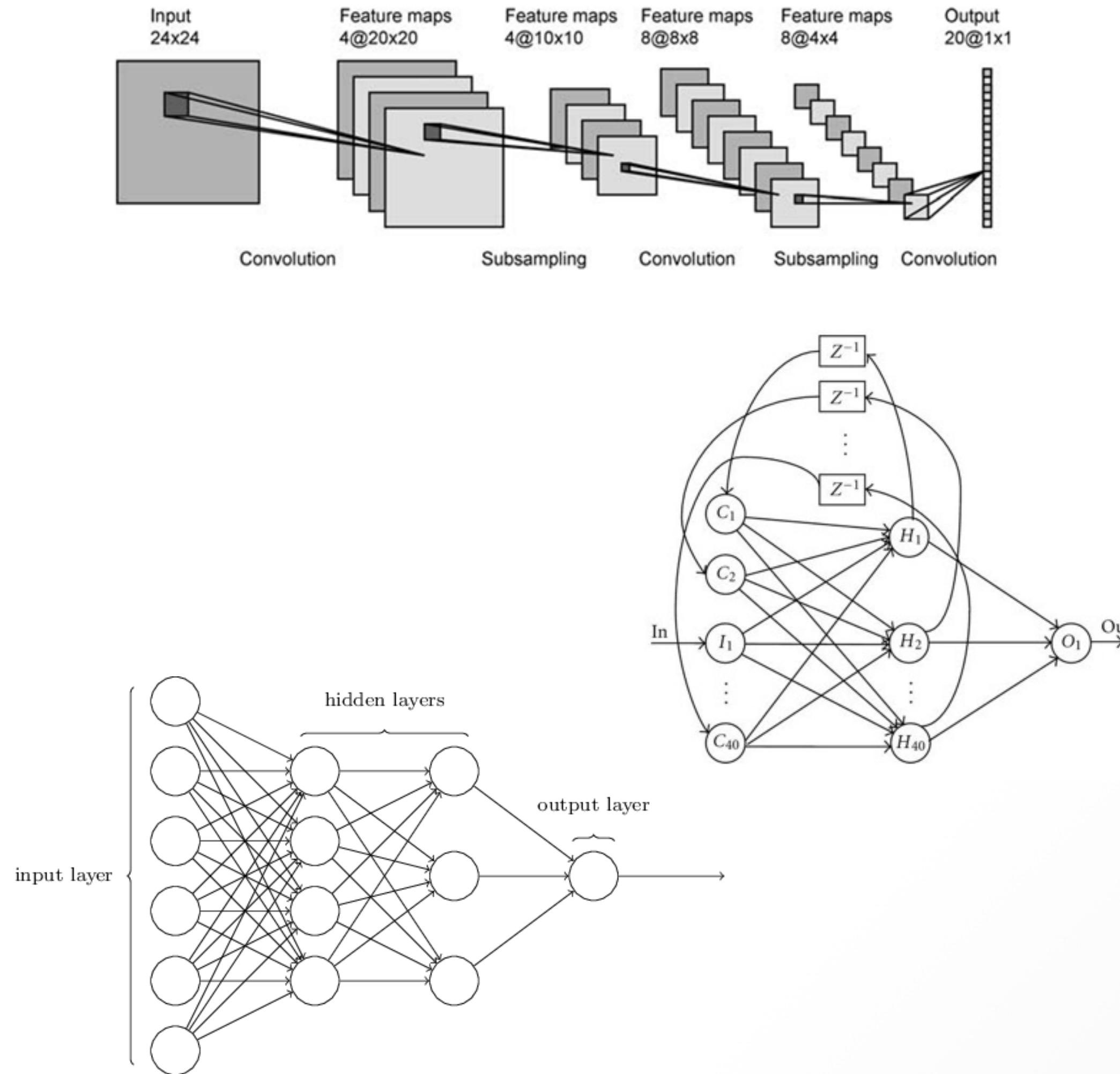


Deep Water

- Native implementation of Deep Learning models for GPU-optimized backends (mxnet, Caffe, TensorFlow, etc.)
- State-of-the-art Deep Learning models trained from the H2O Platform
- Provides an easy to use interface to any of the Deep Water backends.
- Extends the H2O platform to include Convolutional Neural Nets (CNNs) and Recurrent Neural Nets (RNNs) including LSTMs

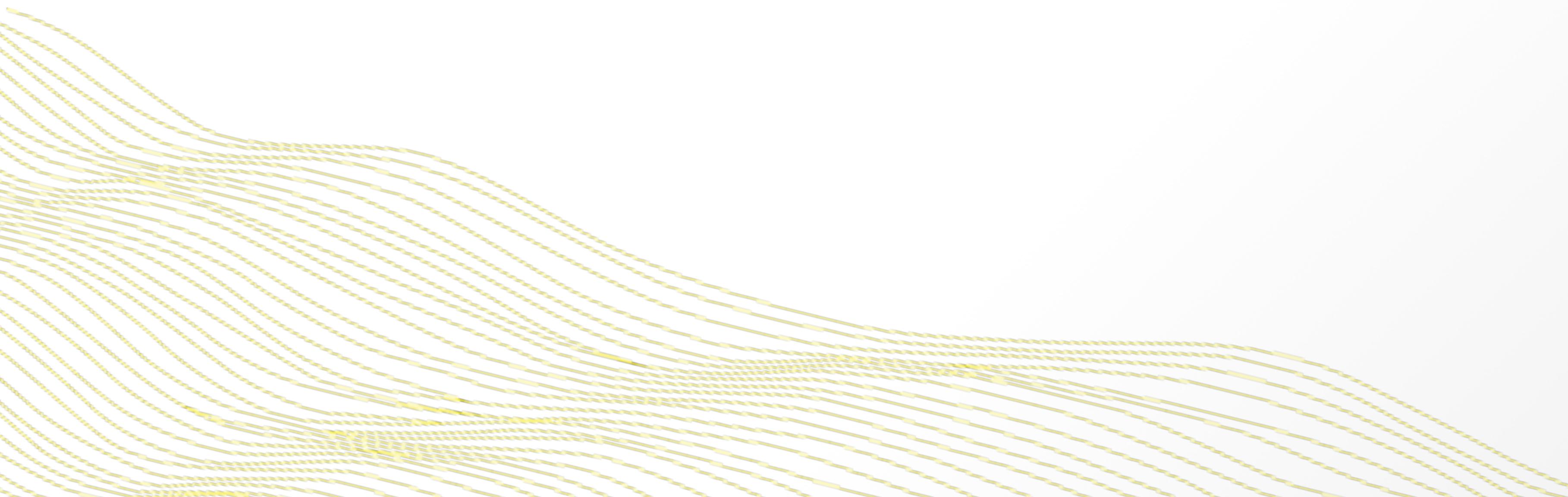
<https://github.com/h2oai/deepwater>

Deep Water Neural Architectures



- » Convolutional Neural Networks (CNNs), which are popular for image data.
- » Recurrent Neural Networks (RNNs), including Long-Short-Term-Memory (LSTMs) for sequence learning including text, audio and video.
- » Multilayer Perceptrons (MLPs), fully connected multilayer artificial neural networks, useful for numeric data.

RSparkling



H2O on Spark



Sparkling Water

- Sparkling Water is transparent integration of H2O into the Spark ecosystem.
- H2O runs inside the Spark Executor JVM.

Features

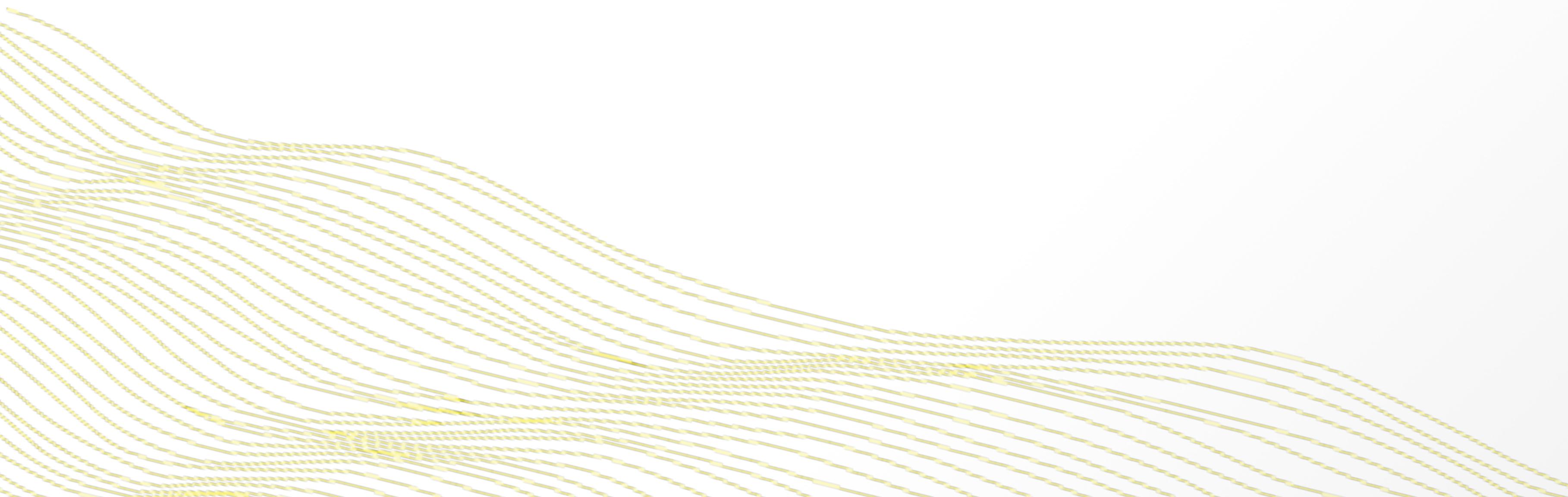
- Provides access to high performance, distributed machine learning algorithms to Spark workflows.
- Alternative to the MLlib/SparkML library in Spark.

rsparkling

- This provides an interface to H2O's machine learning algorithms on Spark, using R.
- This is an extension package for RStudio's sparklyr package that creates an R front-end for a Spark package (e.g. Sparking Water).
- This package implements only the most basic functionality (creating an H2OContext, showing the H2O Flow interface, and converting a Spark DataFrame to an H2OFrame or vice versa).

<http://tinyurl.com/rsparkling-branch>

AutoML



H2O AutoML

- AutoML stands for “Automatic Machine Learning”
- The idea here is to remove most (or all) of the parameters from the algorithm, as well as automatically generate derived features that will aid in learning.
- Single algorithms are tuned automatically using a combination of grid search and Bayesian Optimization algorithms.
- If ensembles are permitted, then a Super Learner will be constructed.

Public code coming soon!