# Ensemble Learning at Scale

## Software, Hardware and Algorithmic Approaches

MLconf

The Machine Learning Conference

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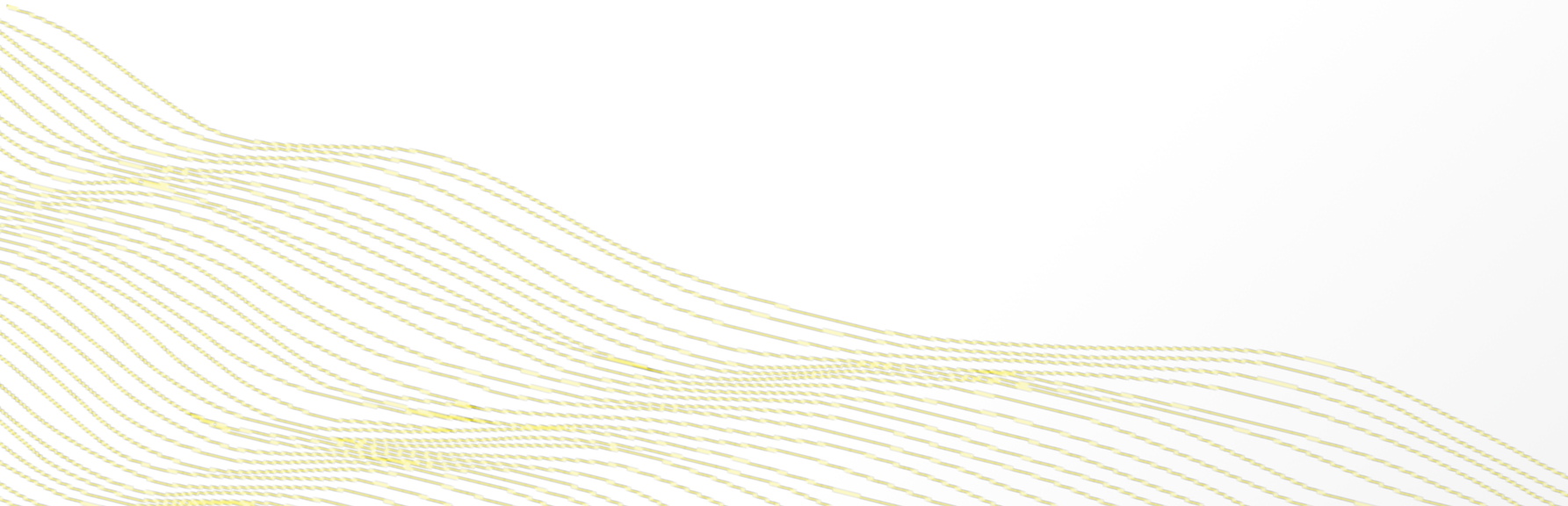
# Introduction

- 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
- Develop open source machine learning software

# Agenda

- Introduction
- Motivation
- Super Learner Algorithm / Stacking
- Subsemble Algorithm
- Online Super Learning
- H2O Ensemble

# Motivation



# Common Types of Ensemble Methods

## Bagging

- Reduces variance and increases accuracy
- Robust against outliers or noisy data
- Often used with Decision Trees (i.e. Random Forest)

## Boosting

- Also reduces variance and increases accuracy
- Not robust against outliers or noisy data
- Flexible – can be used with any loss function

## Stacking

- Used to ensemble a diverse group of strong learners
- Involves training a second-level machine learning algorithm called a “metalearner” to learn the optimal combination of the base learners

# Why Ensembles?

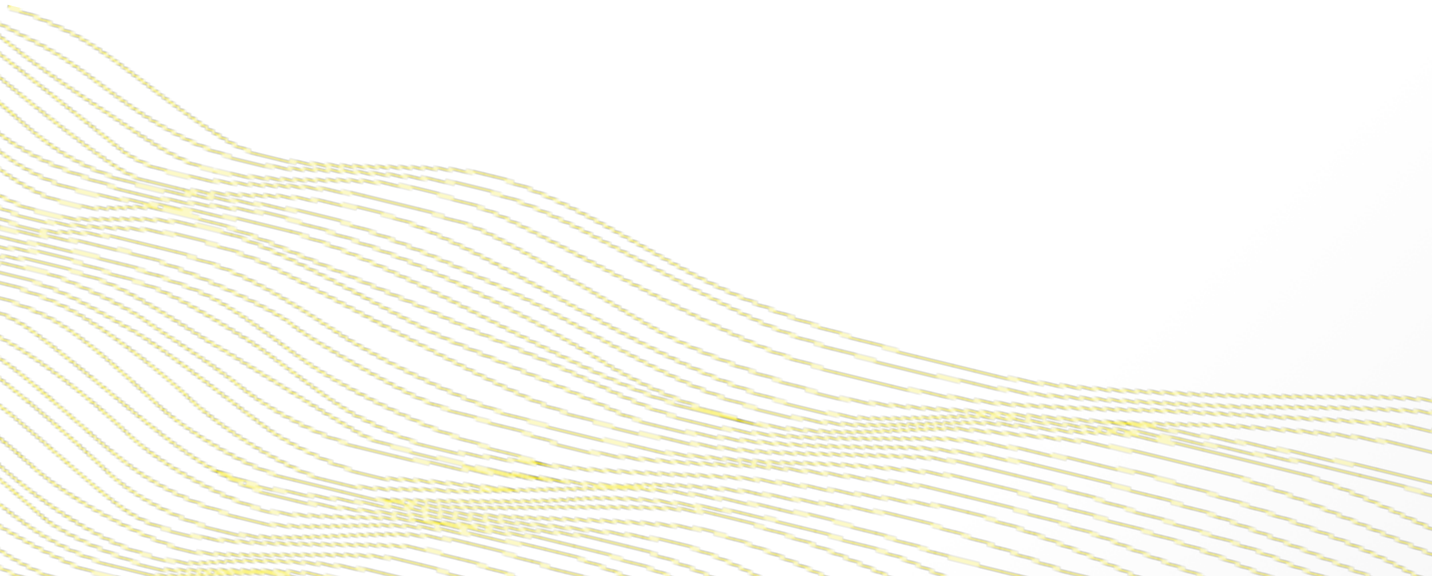
## Strength

- A multi-algorithm ensemble may better approximate the true prediction function better than a single algorithm.
- If model performance is the #1 priority, then multi-algorithm ensembles are a fantastic choice.  This is evidenced by the fact that Stacking wins nearly all Kaggle competitions.

## Weakness

- Increased training & prediction times.
- Increased model complexity.
- Requires large machines or clusters for big data.
- Lack of comprehensive software featuring a large number of algorithms with a single API.

# Super Learner / Stacking



# History of Stacking

## Stacked Generalization

- David H. Wolpert, "Stacked Generalization" (1992)
- First formulation of stacking via a metalearner
- Blended Neural Networks

## Stacked Regressions

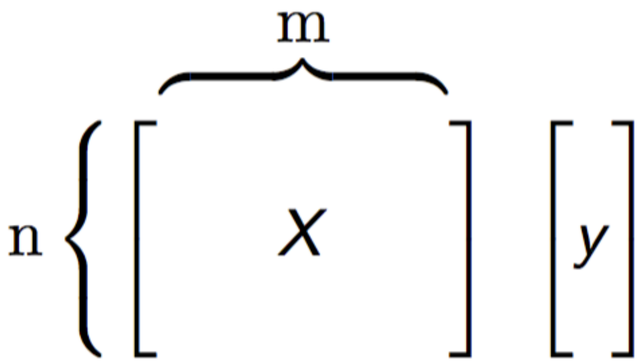
- Leo Breiman, "Stacked Regressions" (1996)
- Modified algorithm to use CV to generate level-one data
- Blended Neural Networks and GLMs (separately)

## Super Learning

- Mark van der Laan et al., "Super Learner" (2007)
- Provided the theory to prove that the Super Learner is the asymptotically optimal combination
- First R implementation in 2010; "SuperLearner" package

# The Super Learner Algorithm

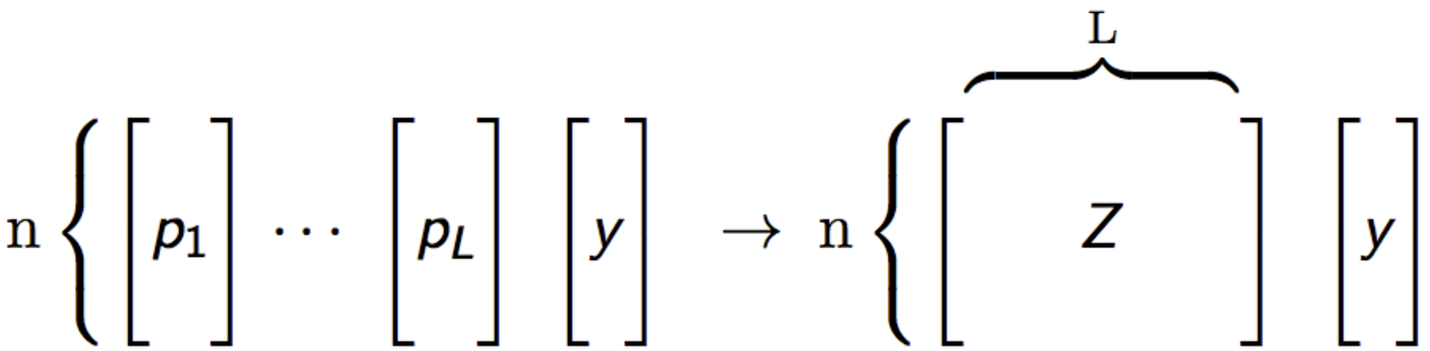
# The Super Learner Algorithm




"Level-zero" data

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

# The 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 ("stack") these prediction vectors together to form a new design matrix, Z.
- Train the metalearner using Z, y.

# Scalable Stacking Solutions

The original SuperLearner R package works well for small datasets, 😄 but not for medium or large datasets. 😞

- Develop alternative formulations of Super Learner than can learn on subsets of the data.
- Use a more scalable language (C++, Java, Scala, Julia) to implement Super Learner.
- Use algorithms that learn iteratively and thus do not need to load the entire training set into memory at once (aka. online learning).

# Scalable Stacking Solutions

## Subsemble

- An R package that implements the Subsemble algorithm for combining models trained on partitions of the data, a variant of Super Learning.
- Like SuperLearner, can be used with any R algorithm.

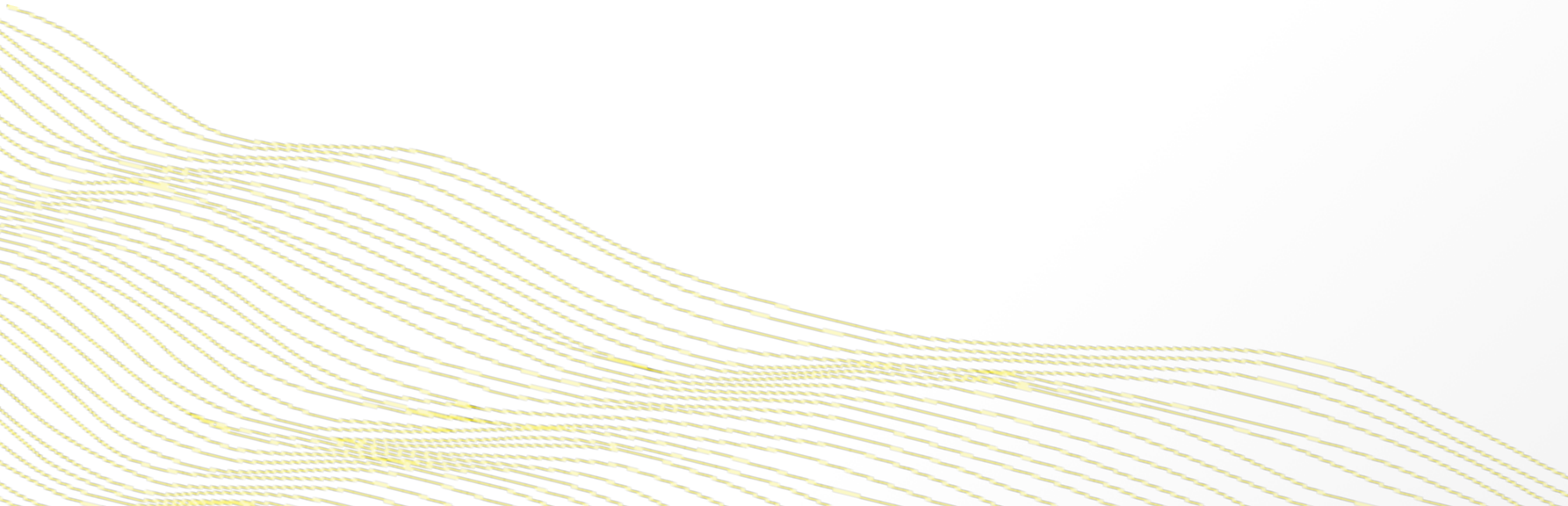
## Online SuperLearner

- Implements an online version of the Super Learner algo.
- Built on top of the out-of-core, online machine learning software, Vowpal Wabbit (VW), in C++.

## H2O Ensemble

- H2O Ensemble implements the standard Super Learner algorithm using H2O distributed algorithms.
- No limit to the size of the cluster that can be used, so it's ideal for datasets bigger than a single node's RAM.

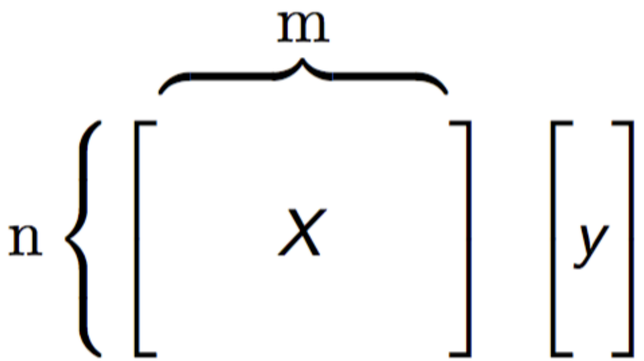
# Subsemble



# The Subsemble Algorithm

- Subsemble is a general subset ensemble prediction method which can be used for small, moderate, or large datasets.
- Subsemble partitions the full dataset into subsets of observations, fits a specified underlying algorithm on each subset, and uses a unique form of k-fold cross-validation to output a prediction function that combines the subset-specific fits.
- An oracle result provides a theoretical performance guarantee for Subsemble.

# The Subsemble Algorithm




"Level-zero" data

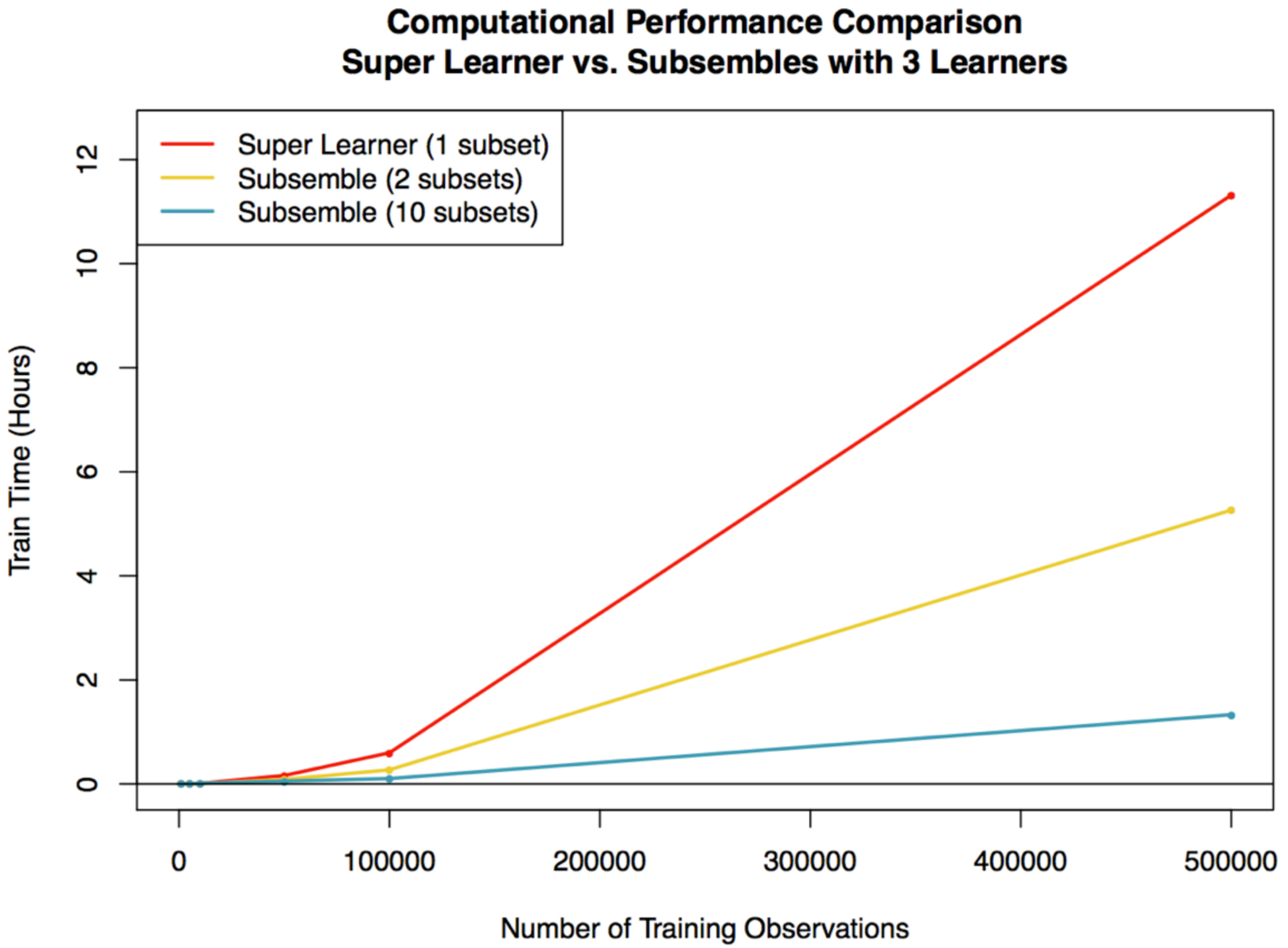
- Start with design matrix, X, and response column, y.
- Specify *L* base learners and a metalearner.
- Partition the data into *J* subsets.
- Partition each subset into *V* folds.
- Note: The $v^{th}$ validation fold spans all *J* subsets.

# Modified K-fold CV in Subsemble

- An example of 5-fold cross-validation for the first subset with a single base learner.
- Even though Subsemble trains models on subsets of the data, it still produces predictions for all *n* rows.
- Instead of producing an *n x L* level-one matrix (as in Super Learner), Subsemble produces an *n x ( J x L )* level-one matrix.

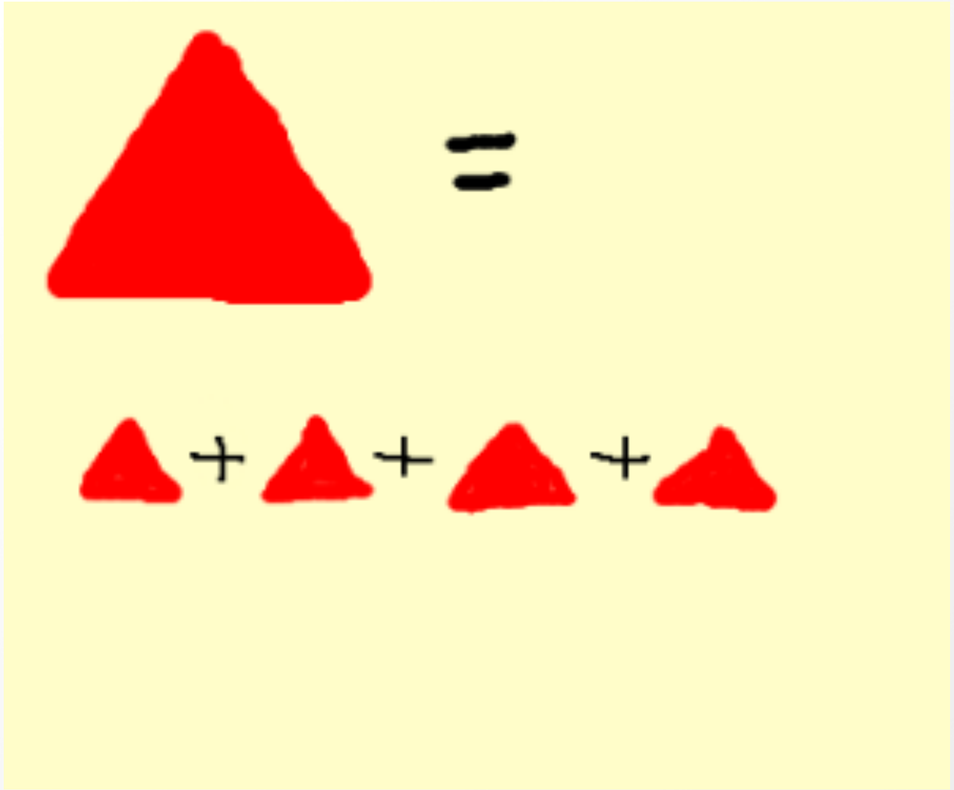
# The Subsemble Algorithm

- An example of training time for a Super Learner and a Subsemble using the same three base learners.
- These were run on a 32-core machine, such that all the base (sub)models could be trained in parallel.
- These benchmarks were executed using the subsemble R package.



# The Subsemble Algorithm

- Subsemble allows you to “squeeze” the machine learning task into pieces small enough to run on your hardware – just select the appropriate number of partitions (subsets).
- If you have heterogenous training data, you may choose to partition your data into subsets using a clustering algorithm.
- There is an extension of the Subsemble Algorithm called “Supervised Regression Tree (SRT) Subsemble Algorithm” which can learn the optimal subsets.



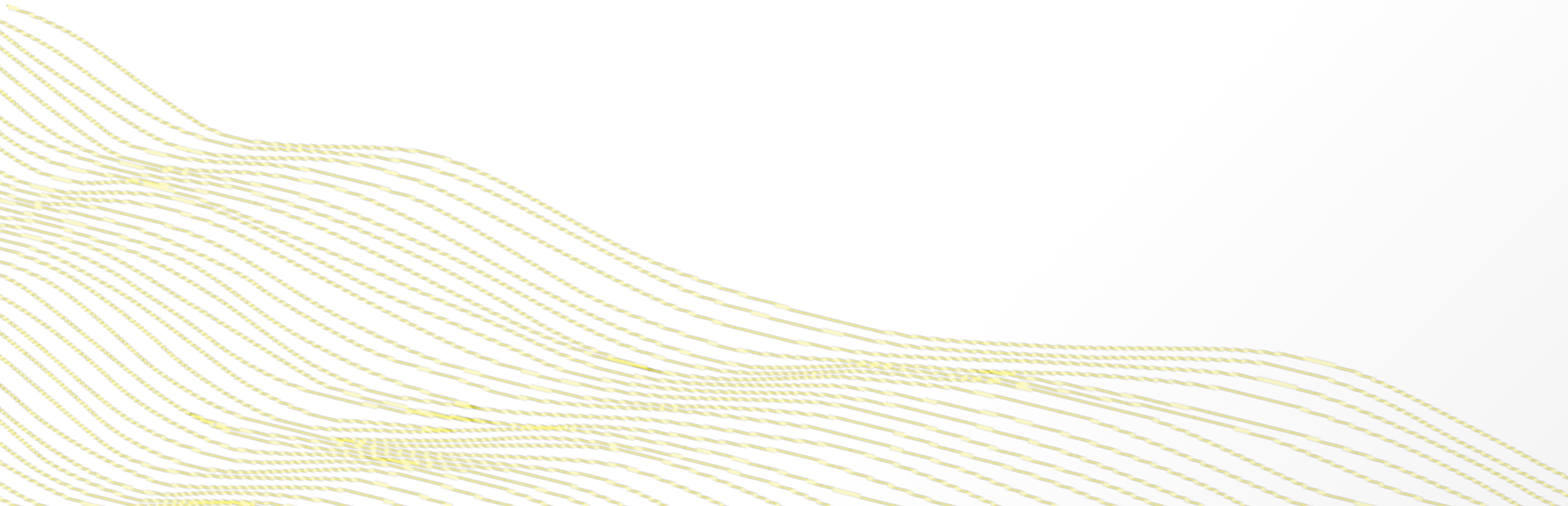
# The Subsemble Algorithm

Stephanie Sapp, Mark J. van der Laan & John Canny.

Subsemble: An ensemble method for combining subset-specific algorithm fits. *Journal of Applied Statistics*, 41(6):1247-1259, 2014.

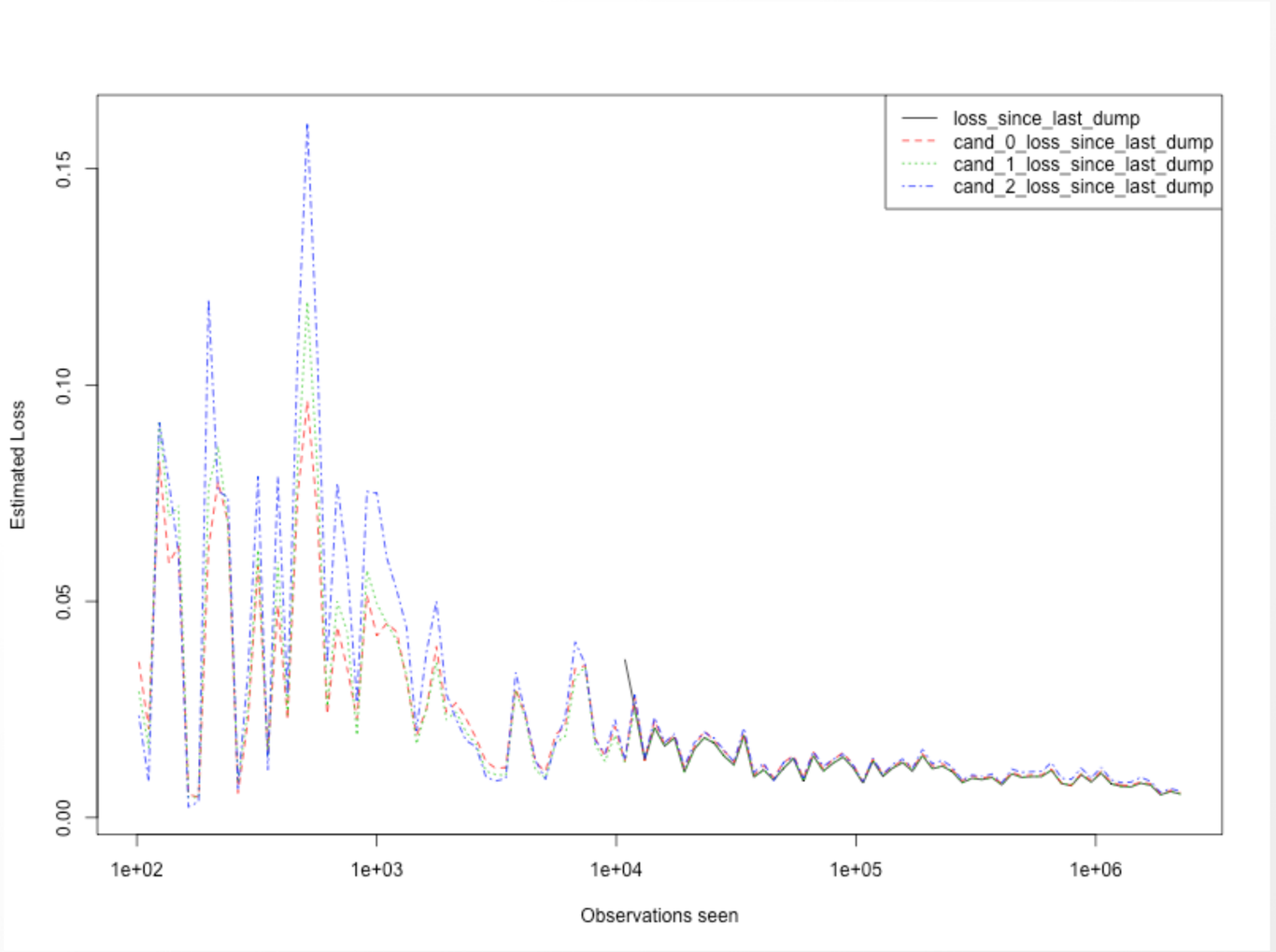
- Article: http://dx.doi.org/10.1080/02664763.2013.864263
- Preprint: https://biostats.bepress.com/ucbbiostat/paper313
- R package: https://github.com/ledell/subsemble

# Online Super Learner



# Online Super Learner

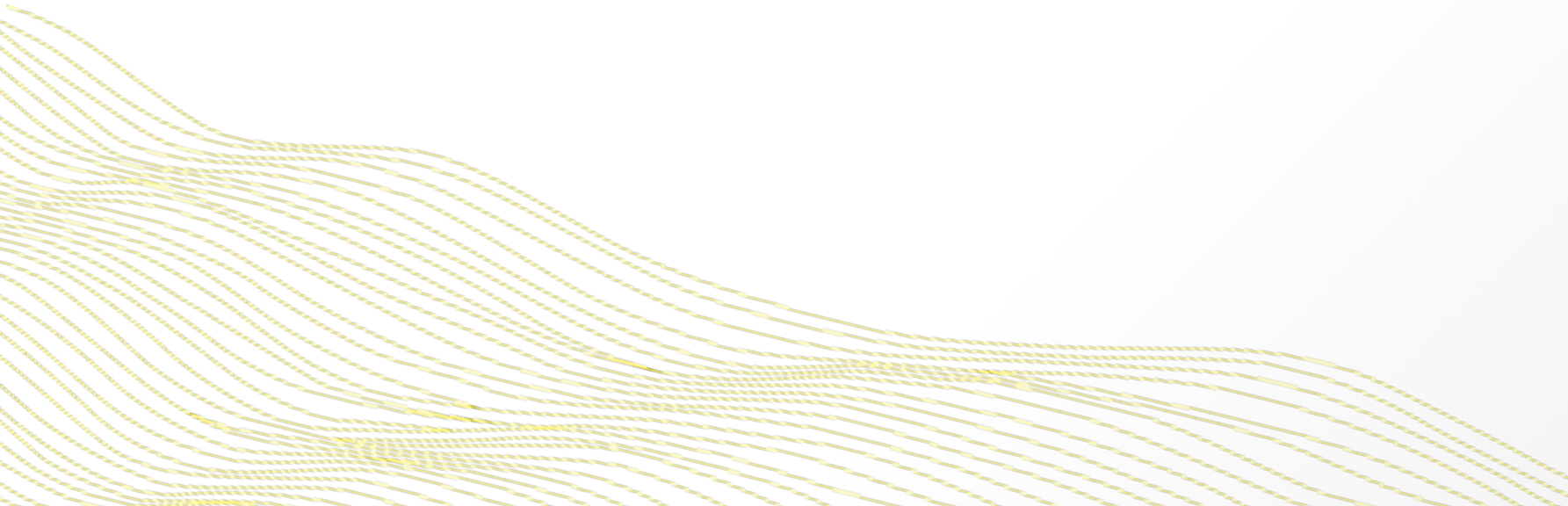
- The “Online Super Learner” is an experiment in extending stacking to an online setting.
- It was implemented on top of Vowpal Wabbit (VW) and uses VW base learners.
- For simplicity, the metalearner is a linear model, trained using the Non-Negative Least Squares (NNLS) algorithm.



# Online Super Learner

- The primary distinction between Super Learner and Online Super Learner is in how the level-one data is generated.
- Single-pass mode: The predicted value for observation *i* is generated using the model trained on observations *1, … , i−1*. These predicted make up the level-one Z matrix.
- Multi-pass mode: Every $v^{th}$ training example is put aside into a hold-out set (never trained on). Each training iteration produ and the predicted values are generated for these samples and placed into the Z matrix.
- The most recent *m* rows of the Z matrix are used to update $\alpha$, the candidate weight vector (in the case of a linear metalearner), which specifies the metalearning fit at a given iteration.

# H2O Ensemble



# H2O Overview

- H2O Ensemble is a scalable implementation of the Super Learner algorithm for H2O.
- H2O is an open-source, distributed machine learning library written in Java with APIs in R, Python, Scala and REST/JSON.
- Produced by H2O.ai in Mountain View, CA.
- H2O.ai advisers are Trevor Hastie, Rob Tibshirani and Stephen Boyd from Stanford.

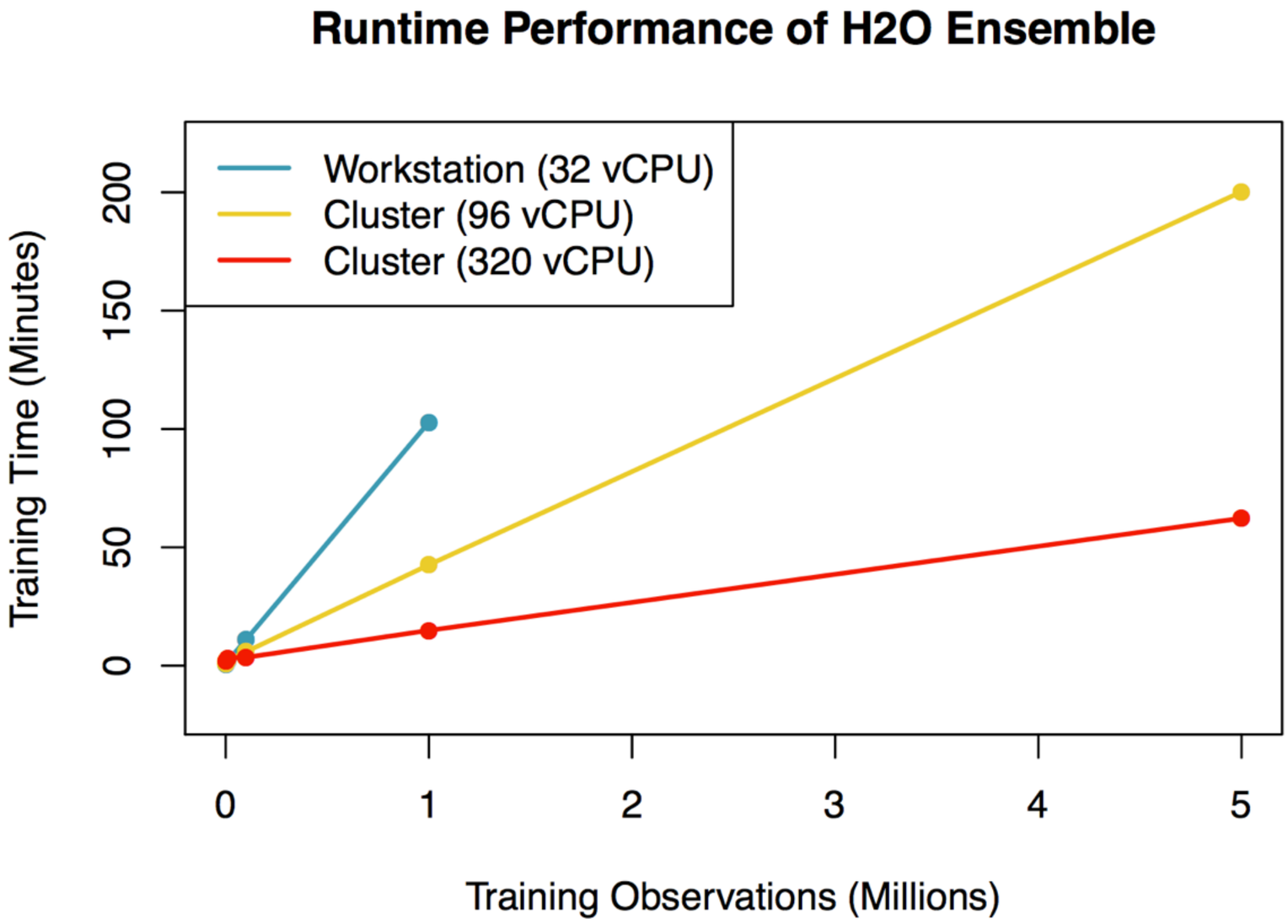

# H2O Ensemble Overview

Using H2O as the base software provides incredible speed-up over R-based packages like SuperLearner and subsemble.

- H2O Ensemble is currently available as an R package, extending the h2o R API, and other APIs are in development.
- Implements regression and binary classification.  Multi-class support is in development.
- Utilities to generate diverse sets of base learners for better performance (e.g. Random Grid Search).

# H2O Ensemble Overview

- To scale, just add nodes to your H2O cluster.
- Also works just as easily on your laptop utilizing all available cores (same software runs single-node and multi-node clusters).



# H2O Ensemble Resources

H2O Ensemble training guide:
http://tinyurl.com/learn-h2o-ensemble

H2O Ensemble homepage on Github:
http://tinyurl.com/github-h2o-ensemble

H2O Ensemble R Demos:
http://tinyurl.com/h2o-ensemble-demos

# Thank you!

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