Become a SUPER LEARNER

Using {sl3} to build ensemble learning models

Kat Hoffman
R-Ladies NYC
September 10, 2019

What is **Ensemble Learning**?

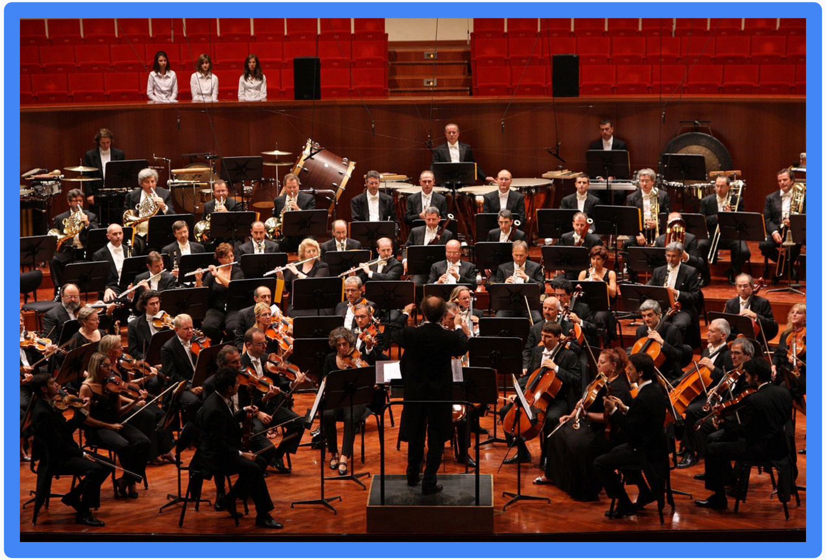

Image source: Royal Philharmonic Society

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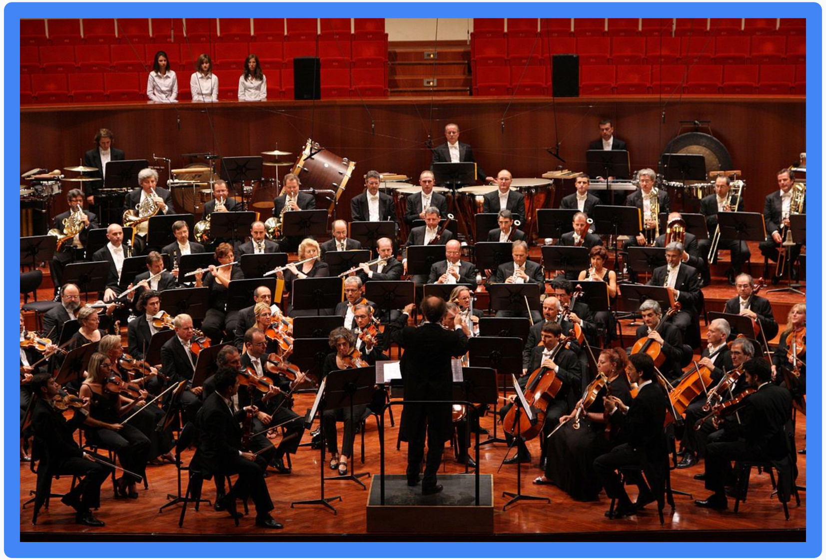

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Ensemble learning: The process of combining multiple models to improve the overall model's prediction performance

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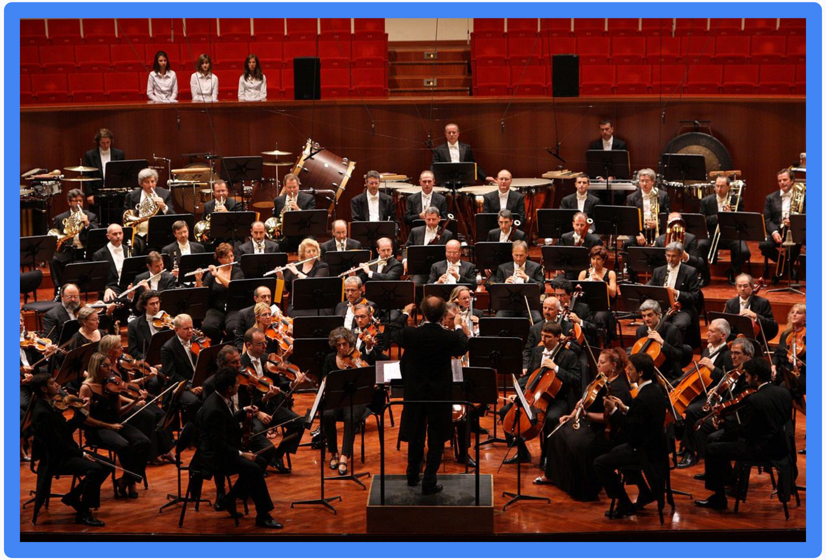

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Common techniques:

1. Bagging
2. Boosting
3. Stacking

Ensembling Technique 1: BAGGING

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Bootstrap Aggregating

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sample data
with replacement

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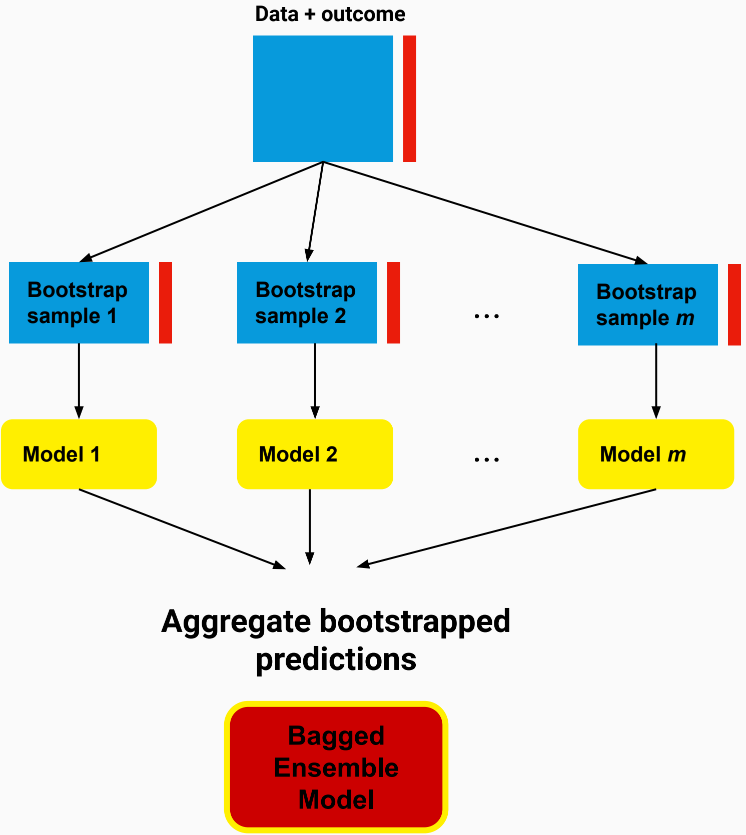

BAGGING with Decision Trees

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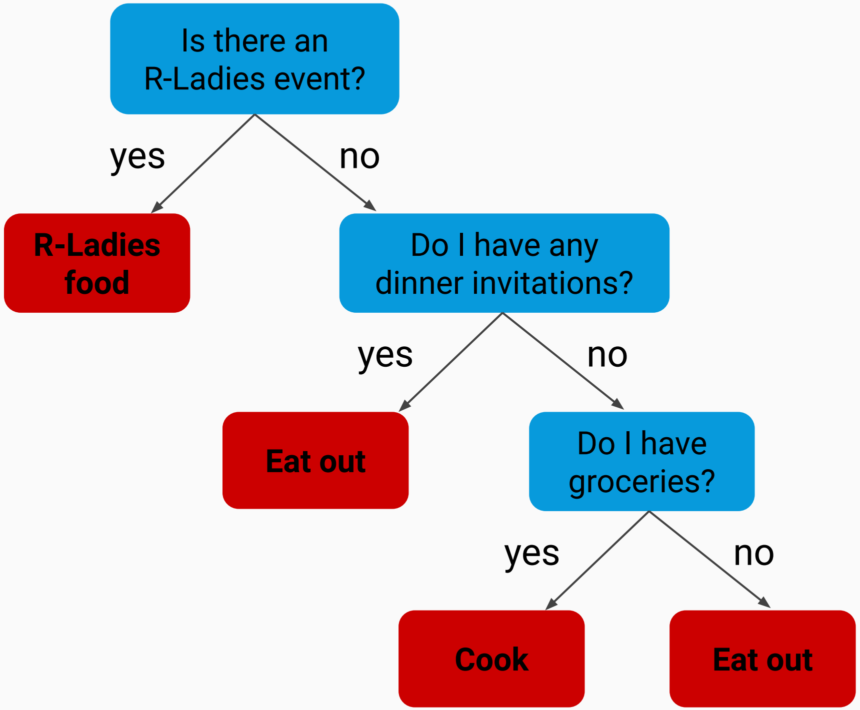
A decision tree for the categorical outcome of:
Dinner Plans



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Decision tree: repeatedly subsetting your data in whichever way best predicts the final outcome

A very common, slight variation of bagging:

Random Forest: aggregated predictions from different decision trees

- Bootstrapped samples (Bagging)
- Limiting and randomizing the predictors to choose from at each decision branch

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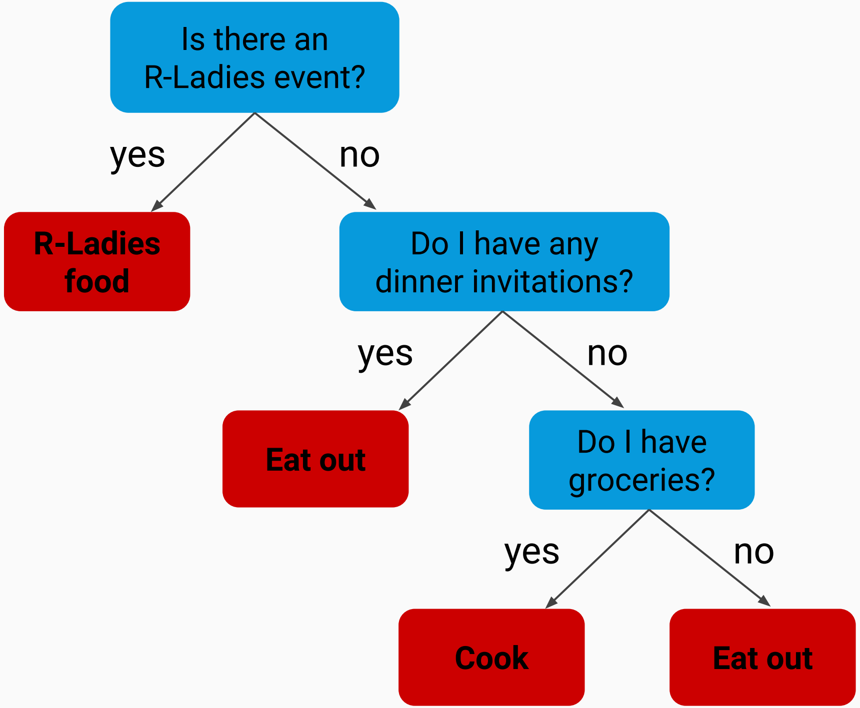

Random Forests in R

- Basic implementation: `RandomForest`
  - Main function: `randomForest()`
  - Simple tuning: `tuneRF()`
- For increased speed and easier tuning of parameters:
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- Well-known interface for many models, not just random forests
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`brickr` + `rayshader` "random forest"
Source: [Twitter, @ryantimpe]

Ensembling Technique 2: BOOSTING

During **bagging**, models are fit ***in parallel***, but in **boosting**, models are fit ***sequentially*** with the goal to learn from past mistakes

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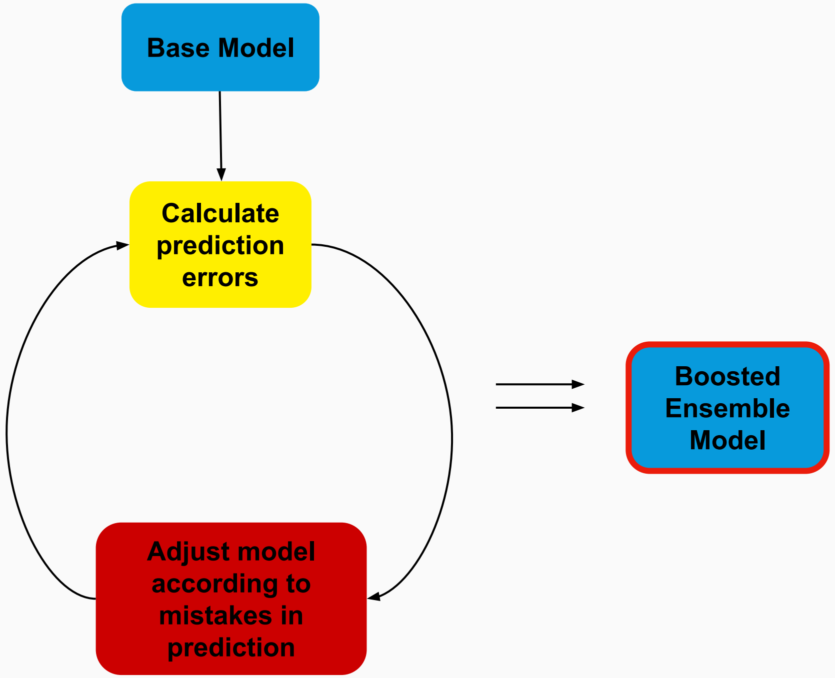

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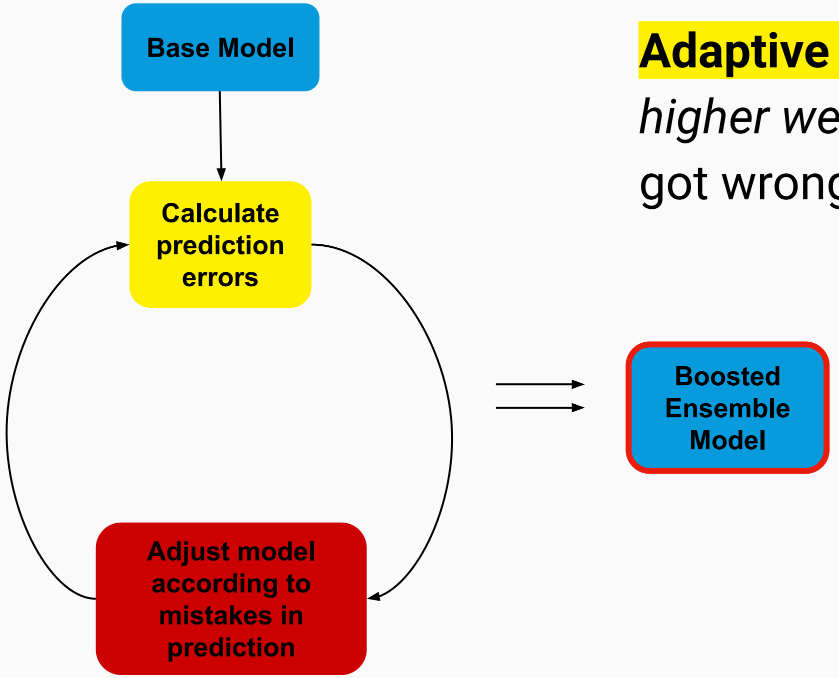

Adaptive boosting: Adjust model by *assigning a higher weight* to the predictions the previous model got wrong

Gradient boosting: Adjust model by *making a new model to predict the errors* of the previous model and adding that error prediction to the previous model

BOOSTING in R

- Adaptive boosting:
  - `Adabag`
- Gradient boosting:
  - `gbm`
  - `Xgboost`
    - Computationally efficient, adds regularization to help with overfitting
- Generalized interface:
  - `caret`
  - `h2o`
  - `mlr/mlr3`

Check out Rika Gorn's slides on **`xgboost`** from her R-Ladies Lightning Talk!

Common Technique 3: STACKING

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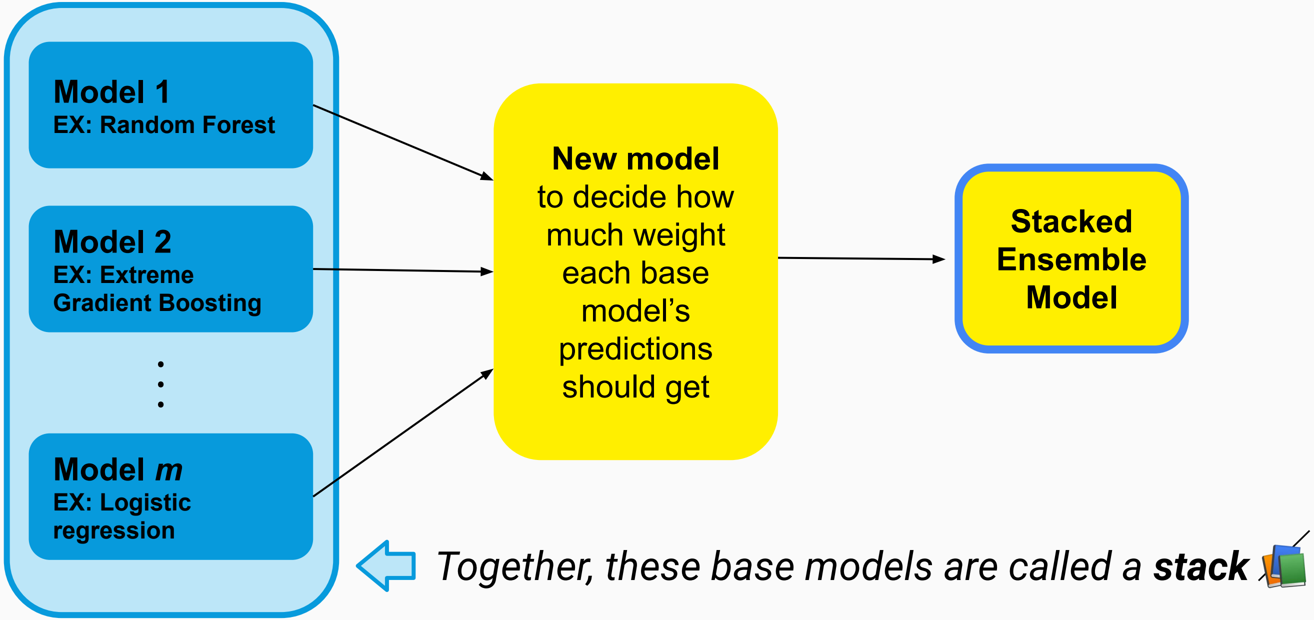

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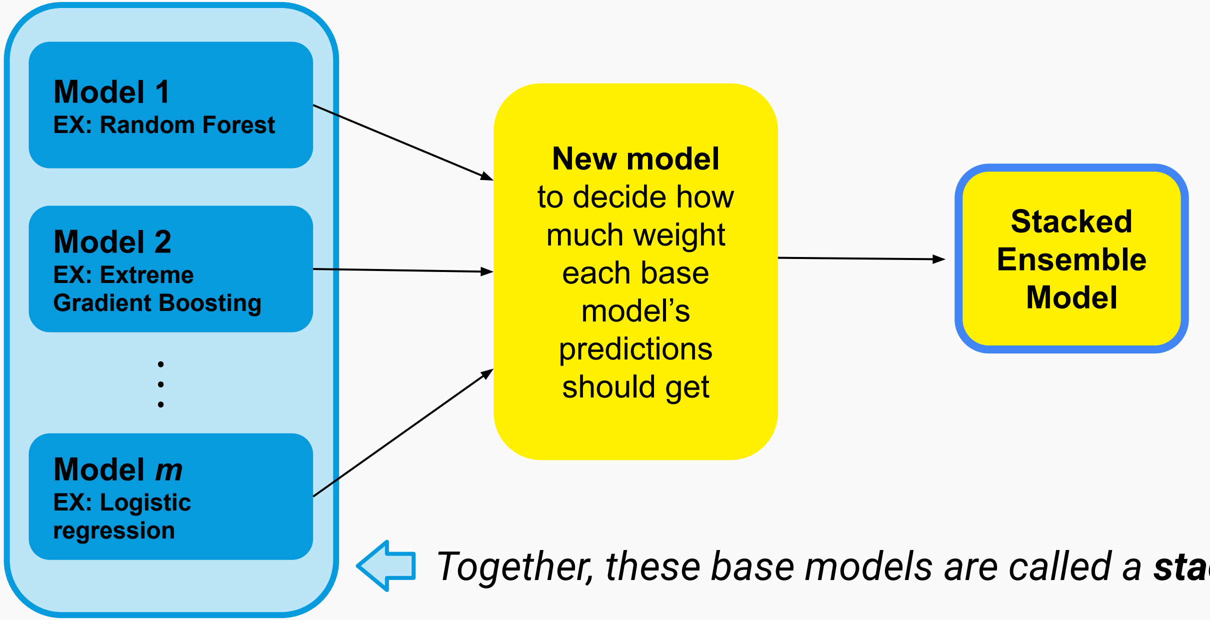

*Together, these base models are called a **stack***

A little jargon:
The base models are often called "**learners**" and the new model is often referred to as the "**meta-learner**"

History of Stacking AKA SUPERLEARNING

Fun stats fact of the day! In the early 2000s, a group of statisticians proved that stacking or "superlearning" would always perform as good or better than the best base model in your stack as sample size approaches ∞

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An important point:

The predictions you input to your meta-learner must come from out-of-sample data (using methods like bootstrapping or cross-validating)

A quick aside: cross-validation

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K-fold cross-validation:

1. splitting your data into equal parts

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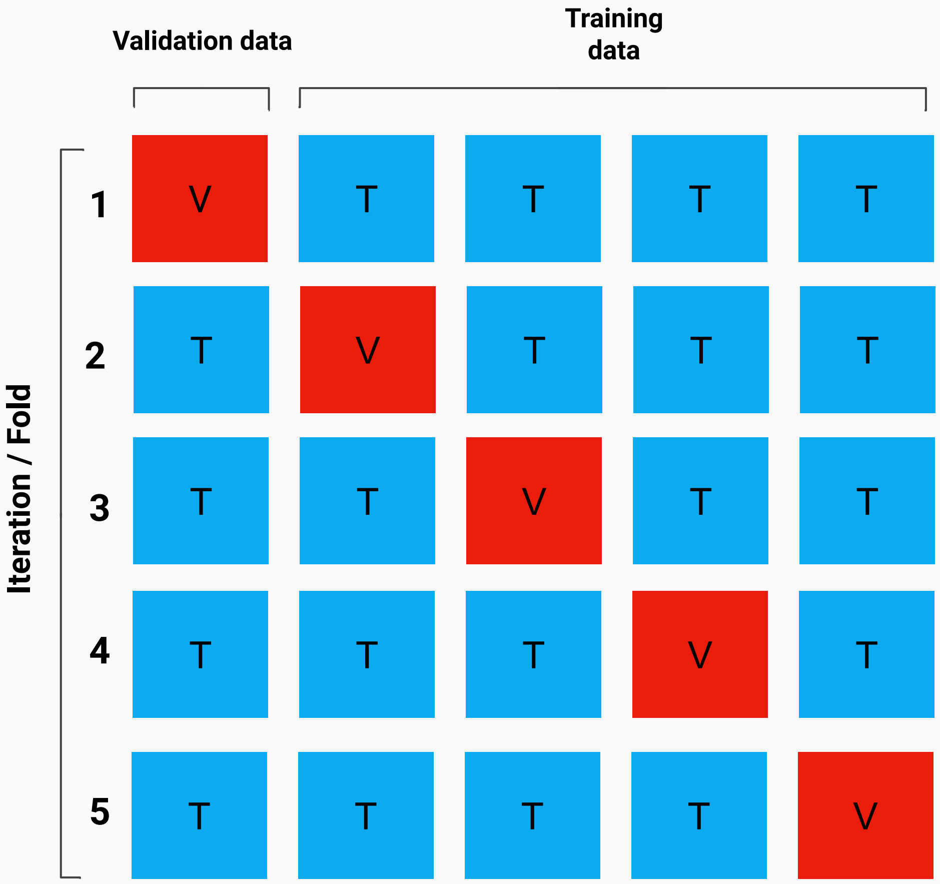
4. Repeating with each piece of data taking its turn as the validation set



Deep Dive of Stacking AKA SUPERLEARNING

One example of a super learner:

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Step 1: Pick base learners

Random Forest

Gradient Boosting Model

Generalized Linear Model

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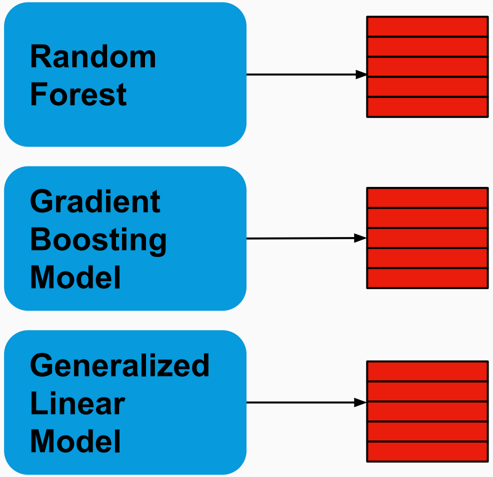

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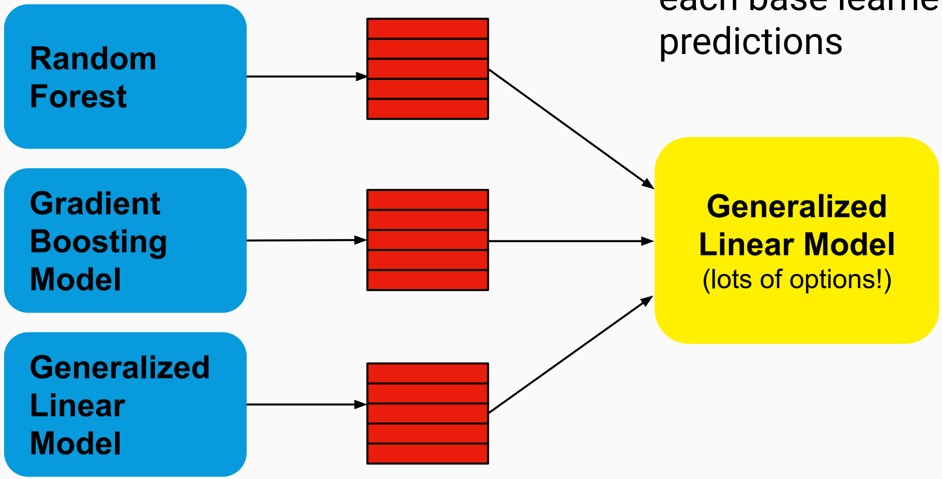

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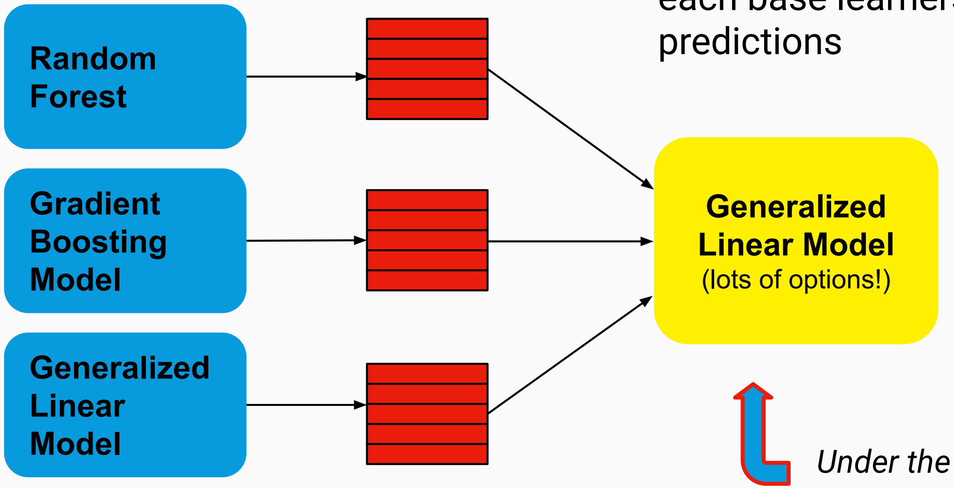

Under the hood:

`True_Outcome ~ RF_pred + GBM_pred + GLM_pred`

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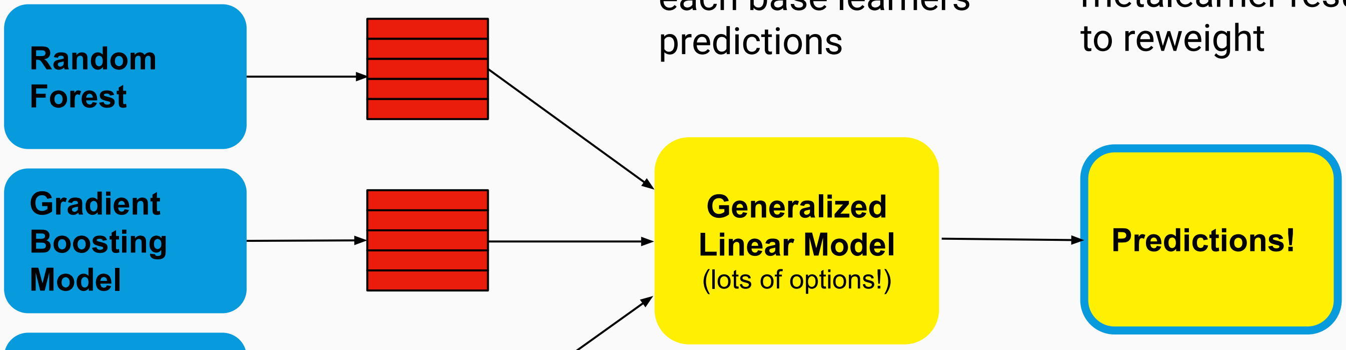

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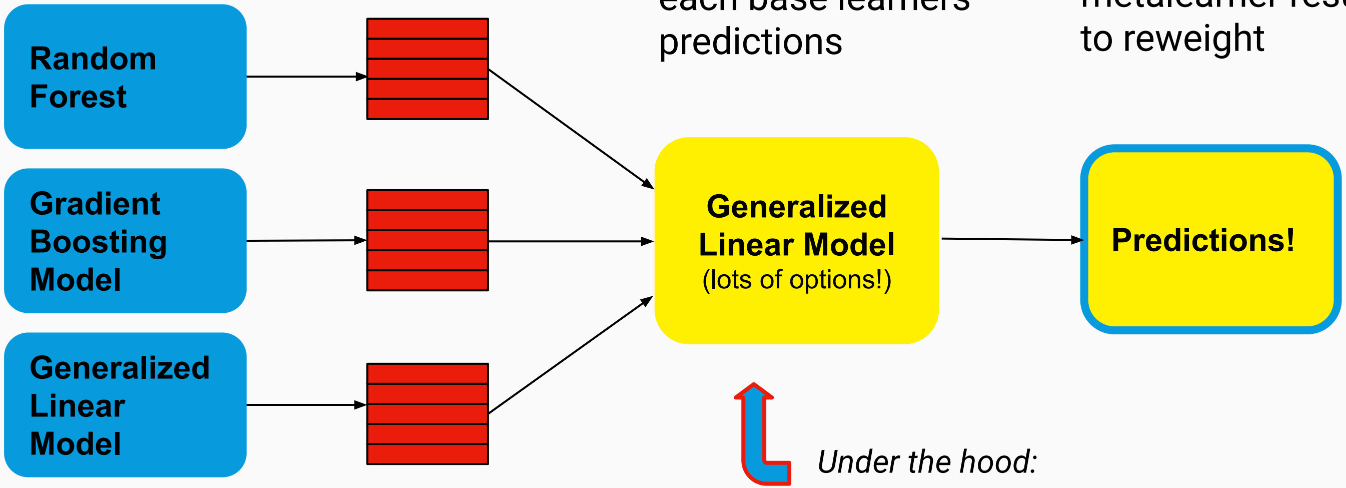

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Stacking AKA SUPERLEARNING in R

There are many packages in `R` to implement stacking/ Superlearning. Some examples:

- `SuperLearner`
- `mlr / mlr3`
- `caretEnsemble`
- `h2o`

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Why `sl3`?

- Comprehensive, faster, modernized syntax update to the older `SuperLearner` package
- Open source, written entirely in `R`
- Syntax modeled after popular machine learning packages such as scikit-learn

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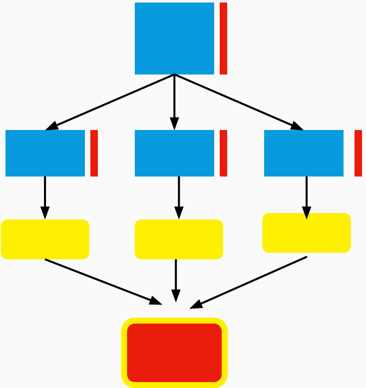
`s13` Demo

WASH Benefits data set: measures of water quality, sanitation, hand washing, and nutritional interventions in rural Bangladesh and Kenya

We will use it to predict: children’s weight-to-height z-scores

SuperReview:

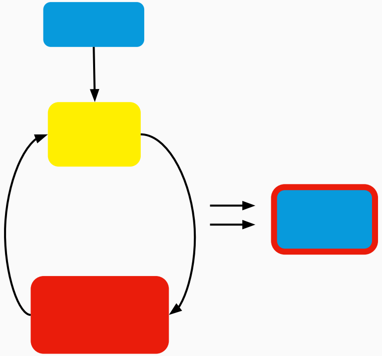
BAGGING



Aggregating bootstrapped predictions

`RandomForest`
`ranger`

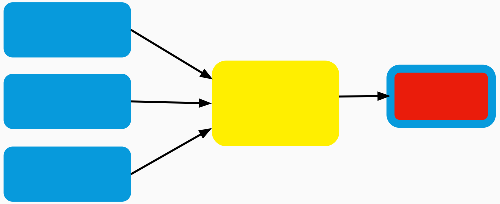
BOOSTING



Sequentially correcting models' mistakes

`AdaBoost`
`gbm`
`xgboost`

STACKING / SUPERLEARNING



Using a new model to blend together base models

`caretEnsemble`
`mlr/mlr3`
`h2o`

`sl3`

Fast, modern update to `SuperLearner` package

Similar syntax to popular machine learning packages in other languages

Written entirely in **R**, contributions welcomed

Helpful Resources:

Ensemble Learning:

- *Towards Data Science* articles:
  - "Understanding Random Forests"
  - "Ensemble Methods: Bagging, Boosting and Stacking"

- Bradley Boehmke's "Hands on Machine Learning with R," Chapters 10-15

- Datacamp's course: "Machine Learning with Tree-Based Models in R"

- Erin Ledell's "Introduction to Practical Ensemble Learning"

Superlearning and `sl3`:

- Teaching materials from the authors of sl3:
  - https://tlverse.org/tlverse-handbook/ensemble-machine-learning.html
  - https://tlverse.org/acic2019-workshop/ensemble-machine-learning.html
  - https://github.com/tlverse/sl3_lecture

- Peterson and Balzar's Causal Inference Seminar, Lab #3: "Super Learner" https://www.ucbbiostat.com/labs

- Polley, Eric C. and van der Laan, Mark J., "Super Learner In Prediction" (May 2010). *U.C. Berkeley Division of Biostatistics Working Paper Series*. Working Paper 266. https://biostats.bepress.com/ucbbiostat/paper266

Special thanks to one of `sl3`'s authors, Nima Hejazi, for answering questions.