DataRobot R Package

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DataRobot

Today’s agenda:

1. What is DataRobot?
   a. A Boston-based software company
   b. A massively parallel modeling engine
   c. An R package (today’s focus)

2. An example to demonstrate the R package:
   a. Predicting compressive strength of concrete
   b. Shows typical DataRobot modeling project
   c. Demonstrates partial dependence plots

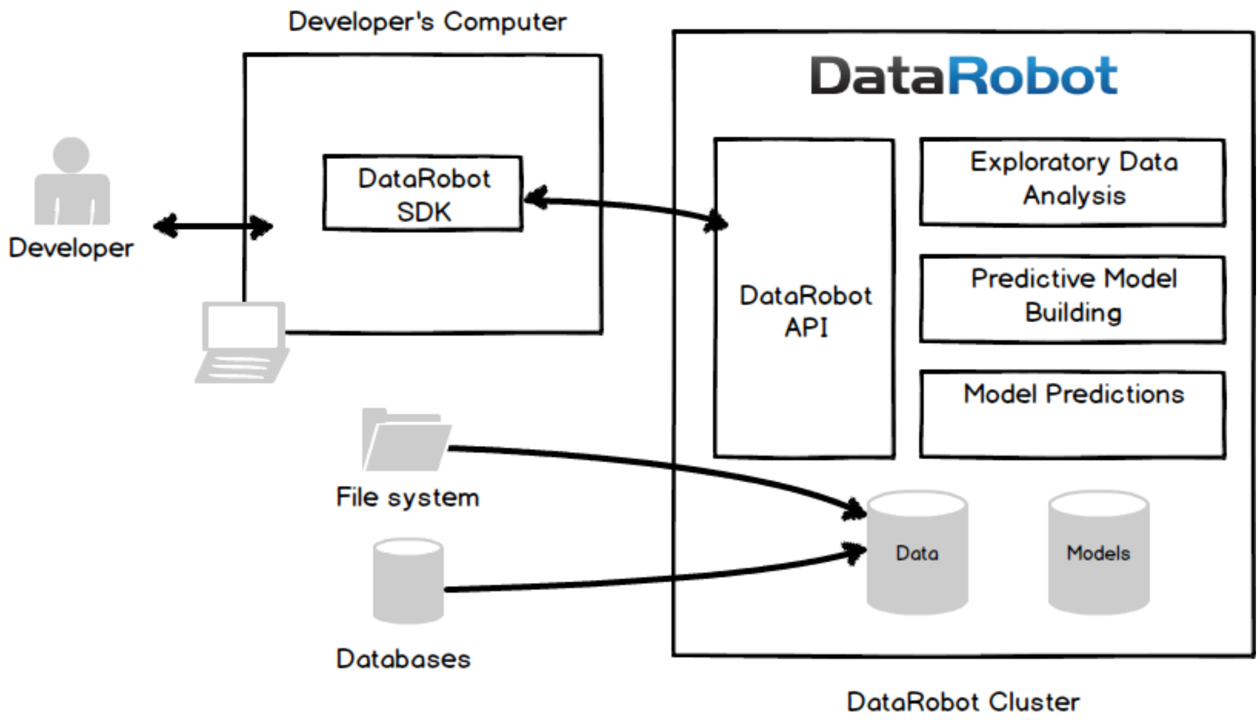
What is DataRobot?

1: Boston-based software company

2: Massively parallel modeling engine
- On multiple hardware platforms
- Under various operating systems
- Has many software components:
  - R
  - Python
  - … and various others

API server

3: R API client - the **DataRobot** R package


Developer's Computer
DataRobot
Developer
DataRobot
SDK
DataRobot
API
Exploratory Data
Analysis
Predictive Model
Building
Model Predictions
File system
Data
Models
Databases
DataRobot Cluster

A few key details:

- Package in the final stages of internal testing
- Will be released via R-Forge under the MIT license
- Two vignettes are available with the package:
  - "Introduction to the DataRobot R package"
  - "Interpreting Predictive Models, from Linear Regression to Machine Learning Ensembles"

Today's predictive modeling example:

- Objective: predict the compressive strength of concrete
- Data source: **ConcreteFrame**
- Each record describes one laboratory concrete sample
- Target variable: Strength
- Prediction variables: Age + 7 composition variables

Creating the DataRobot modeling project

1. Upload the modeling dataframe:

   `> MyDRProject <- SetupProject(ConcreteFrame,"ConcreteProject")`

2. Specify the target variable to be predicted and start building models:

   `> StartAutopilot(Target="Strength", Project = MyDRProject)`

3. Add a custom R model to the project:

   `> CreateCustomModel(MyDRProject, LogAgeFit, LogAgePredict, “R:LinearWithLogAge”)`

4. Retrieve the leaderboard summarizing all project models:

   `> ConcreteLeaderboard <- GetAllModels(MyDRProject)`

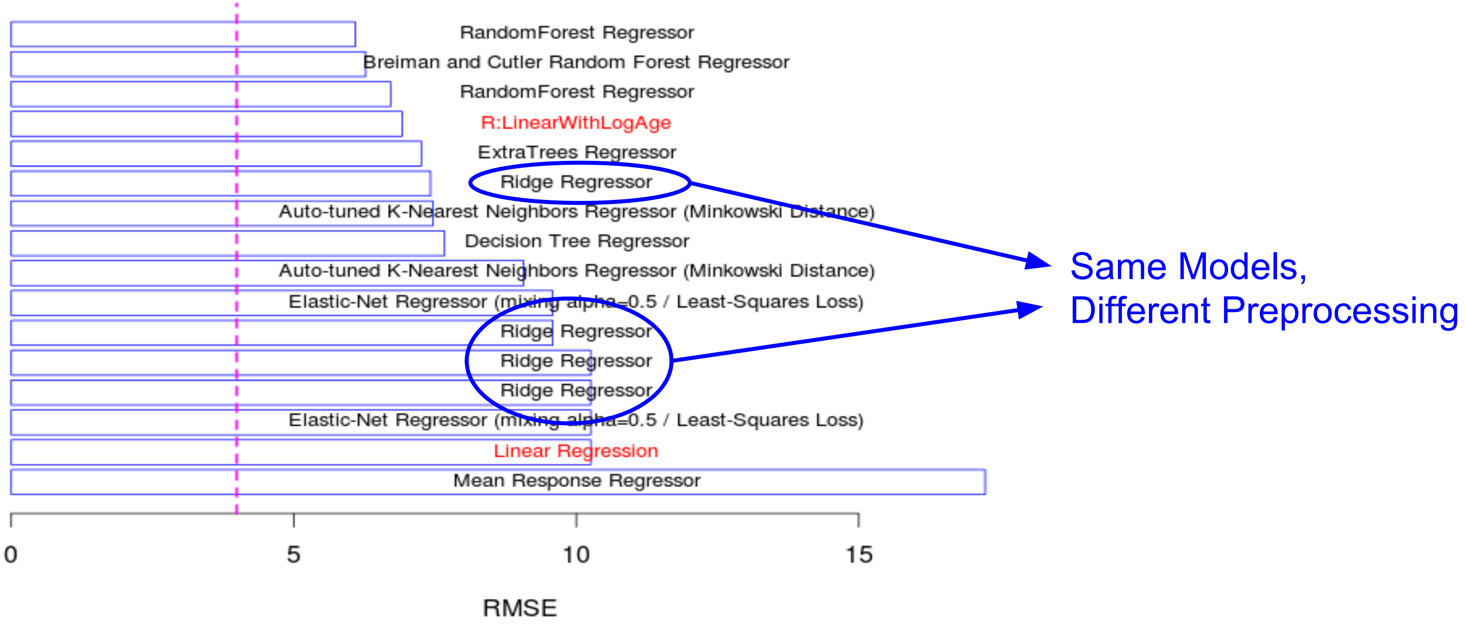
Function arguments for CreateCustomModel

```
LogAgeFit <- function(response, data, extras=NULL){
  #
  DF <- cbind.data.frame(data,
         CustomModelResponseY = response)
  model <- lm(CustomModelResponseY ~ . - Age +
                    log(Age), data = DF)
  return(model)
}
```

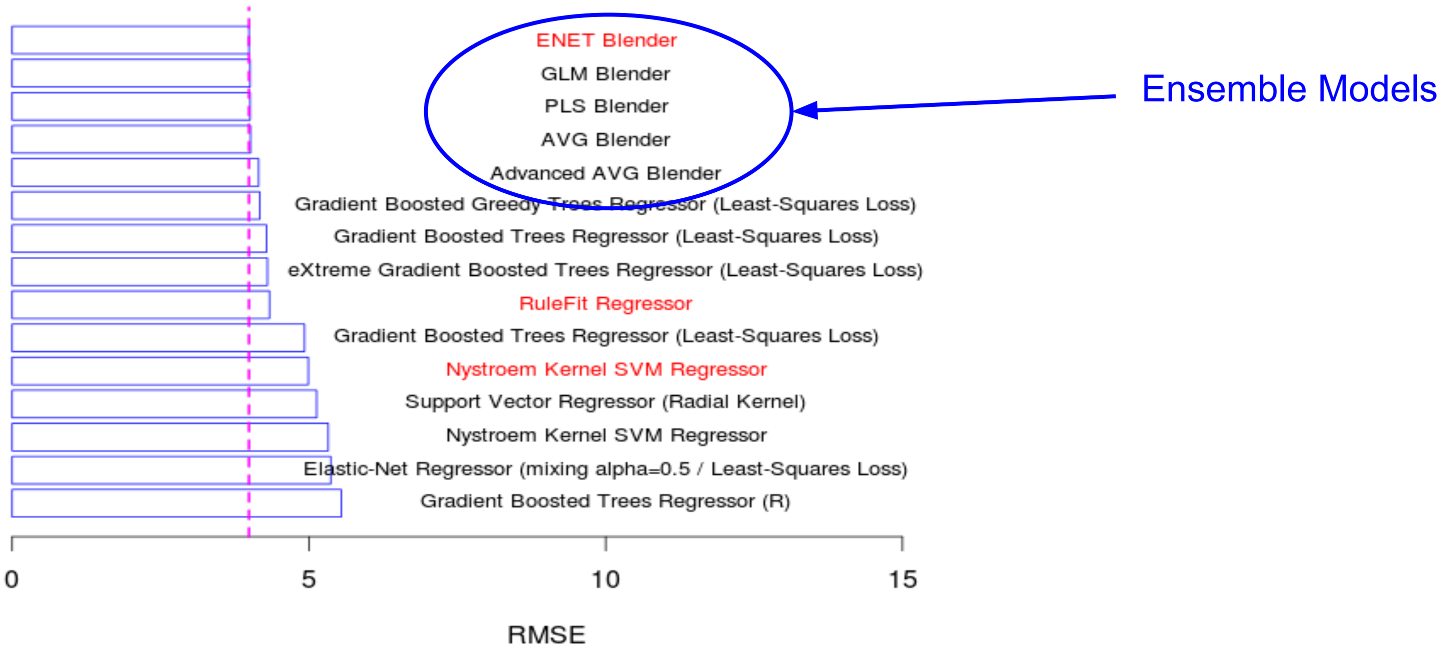
Model fitting function

```
LogAgePredict <- function(model,data){
  predictions <- predict(model, newdata = data)
  return(predictions)
}
```

Prediction function



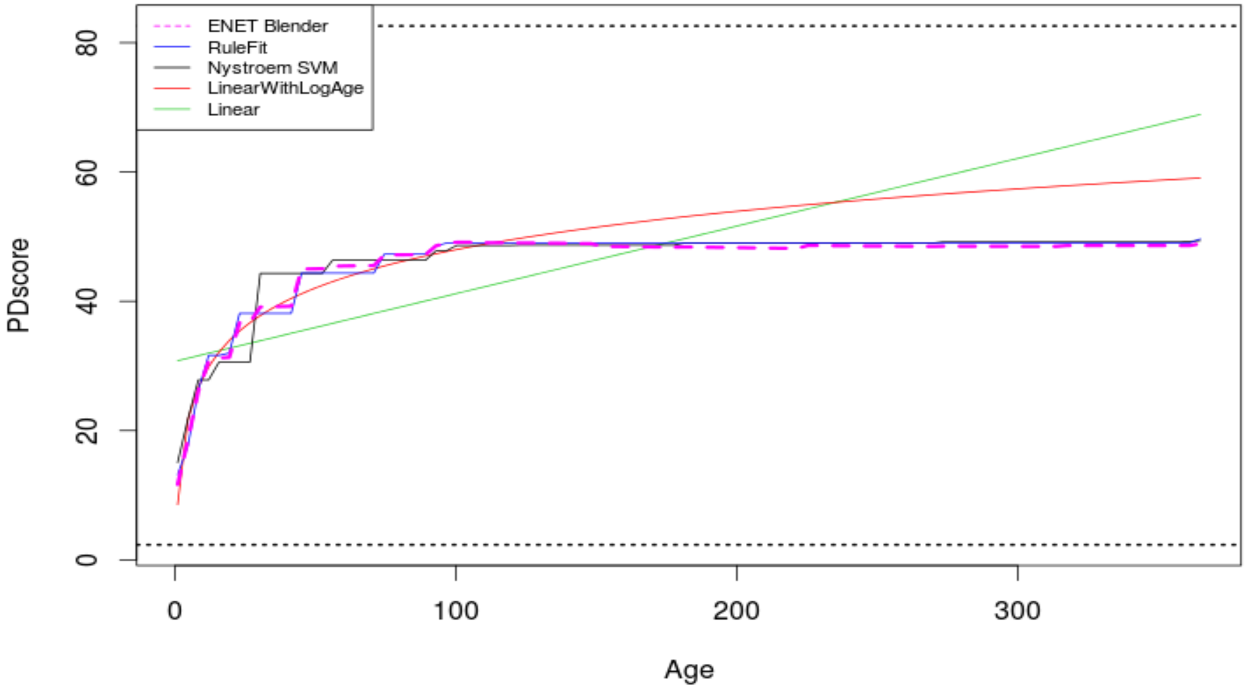
ConcreteLeaderboard: the poorer models (ranks 16-31)



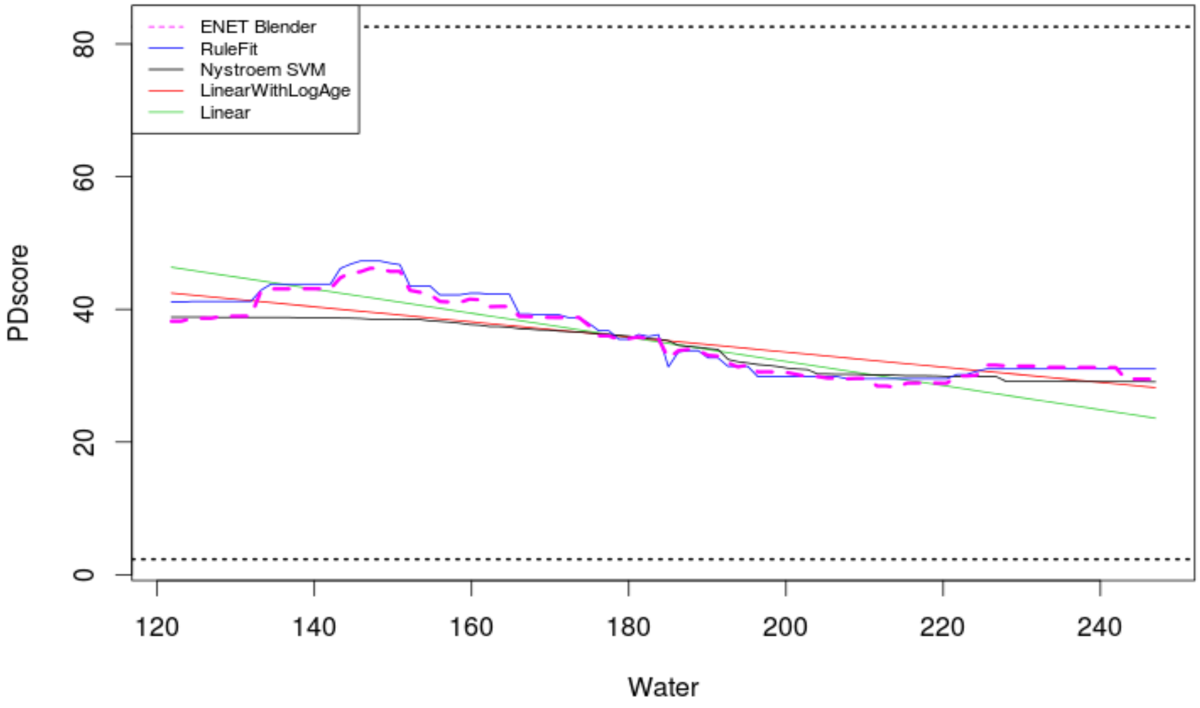
ConcreteLeaderboard: the better models (ranks 1-15)

Understanding complicated models

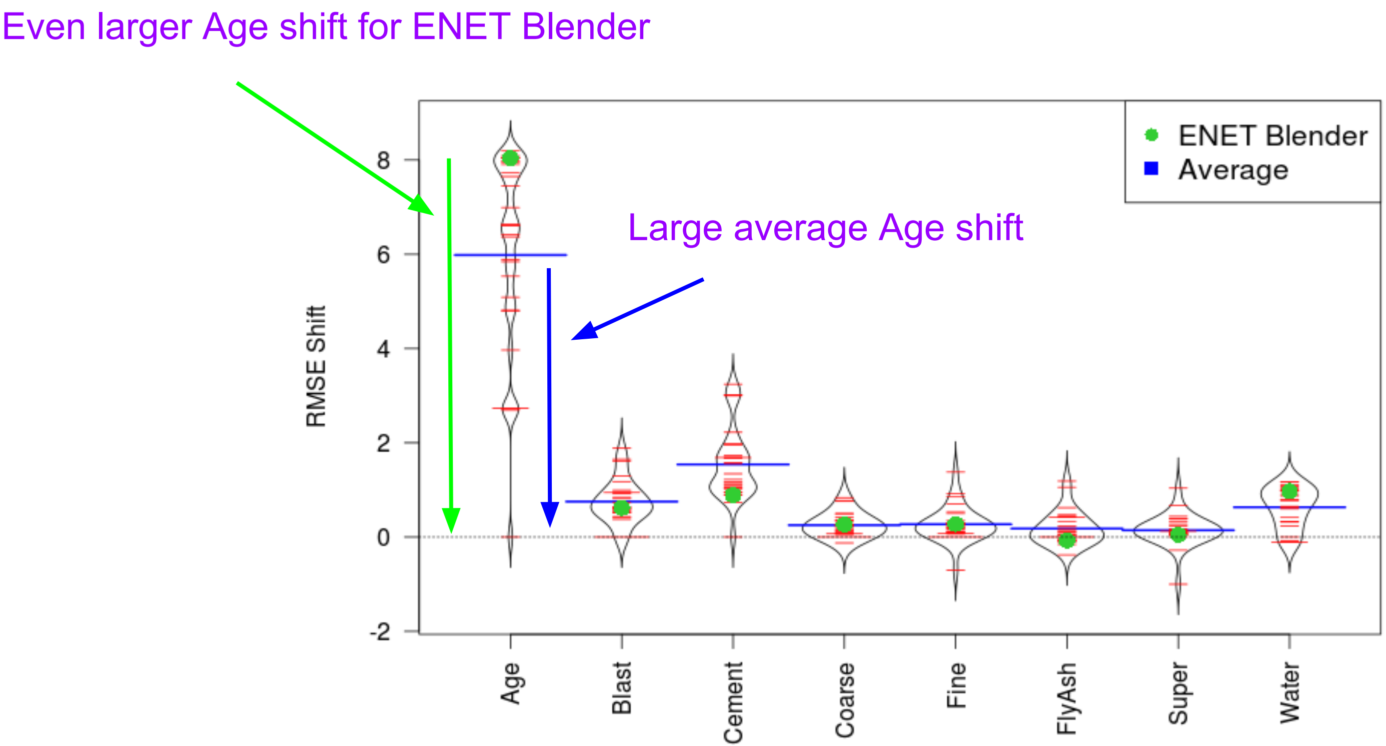
- Linear regression models - easily explained via coefficients
- Not true for random forests, boosted trees, SVMs, etc.
- Alternative: partial dependence plots (Friedman 2001)
    - To assess dependence on x_j, average the predictions over all *other* covariates
    - Compute this average for a representative range of x_j values and plot
    - Linear model: plot is straight line with slope equal to coefficient of x_j



Partial dependence plots for Age



Partial dependence plots for Water



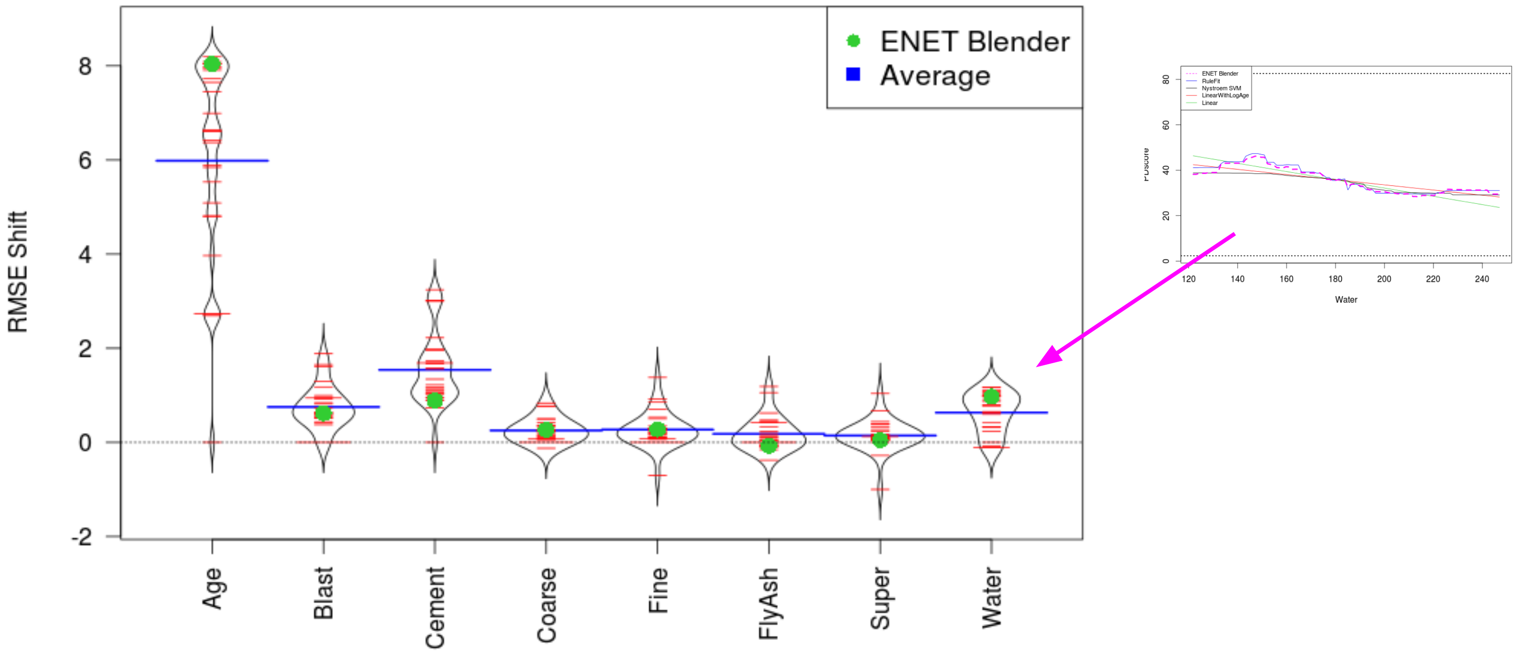
Importance from permutations: large RMSE increase => important variable

Summary of the concrete strength example

- Best model = ENET Blender
  - Age dependence shows nonlinear hard saturation behavior
  - Water dependence is nonlinear and non-monotonic

- Combining with variable importance results:
  - Average measures: Age > Cement > Blast Furnace Slag > Water
  - ENET Blender measures: Age > Water > Cement > Blast Furnace Slag

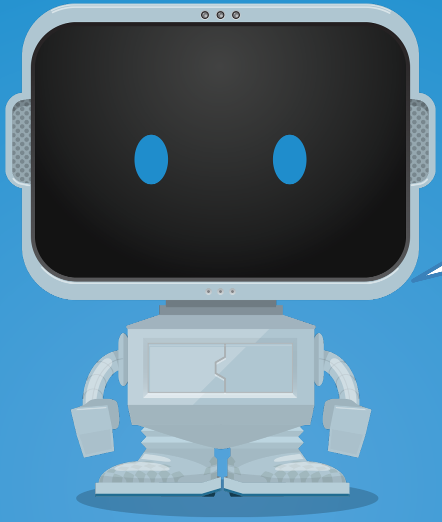
- Best model captures Age saturation behavior and nonmonotonic Water dependence that other models can’t



Note the novel water dependence for the best model

DataRobot

Questions?



Want to use the DataRobot R package?
Email us at:
useR2015@datarobot.com

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Slides available at: bit.ly/UseR2015

Vignette - Intro to DataRobot: bit.ly/1dzgppC

Vignette - Two Applications: bit.ly/1KtWCGI

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