Ideas on Machine Learning Interpretability

Patrick Hall, Wen Phan, SriSatish Ambati and the H2O.ai team

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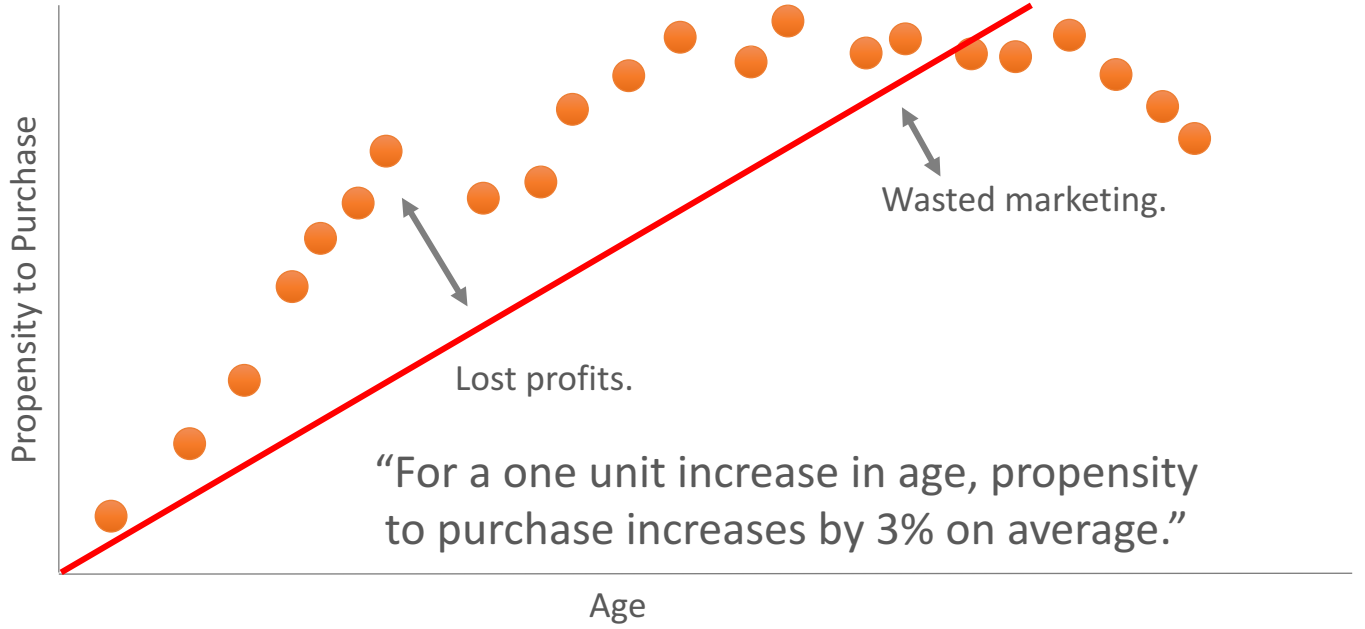
Big Ideas

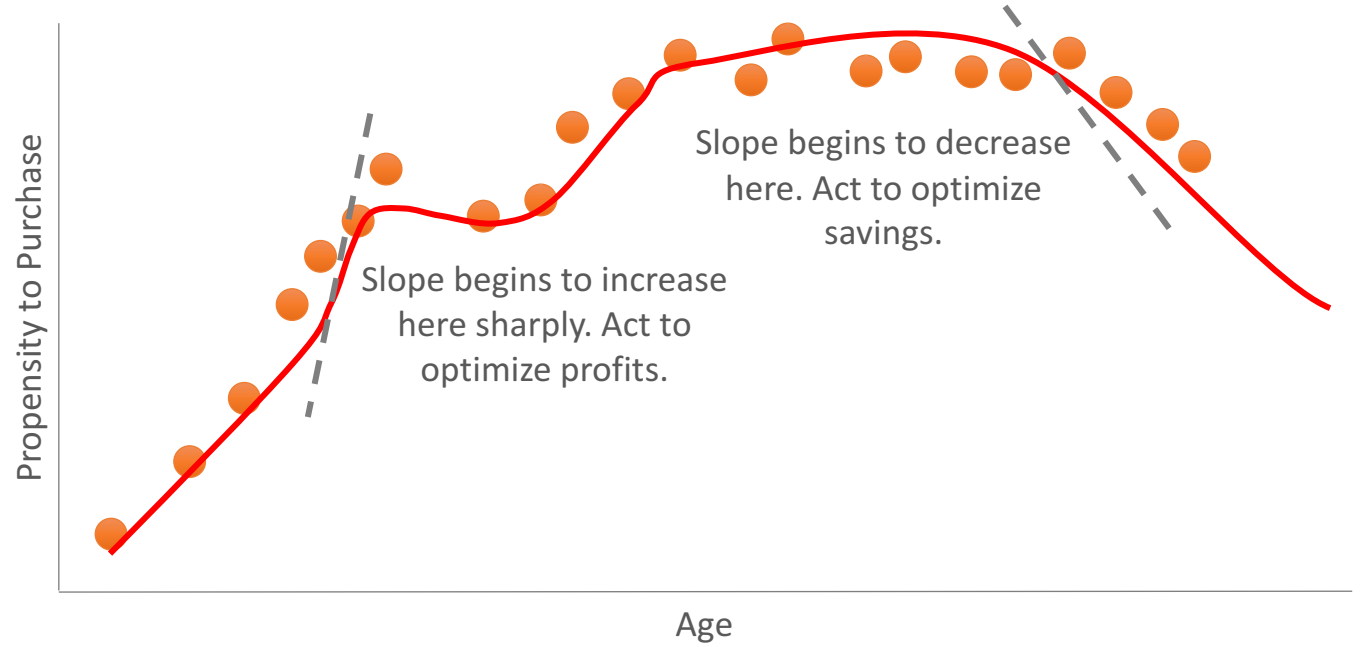
Linear Models

Exact explanations for ***approximate*** models.



Machine Learning

Approximate explanations for ***exact*** models.



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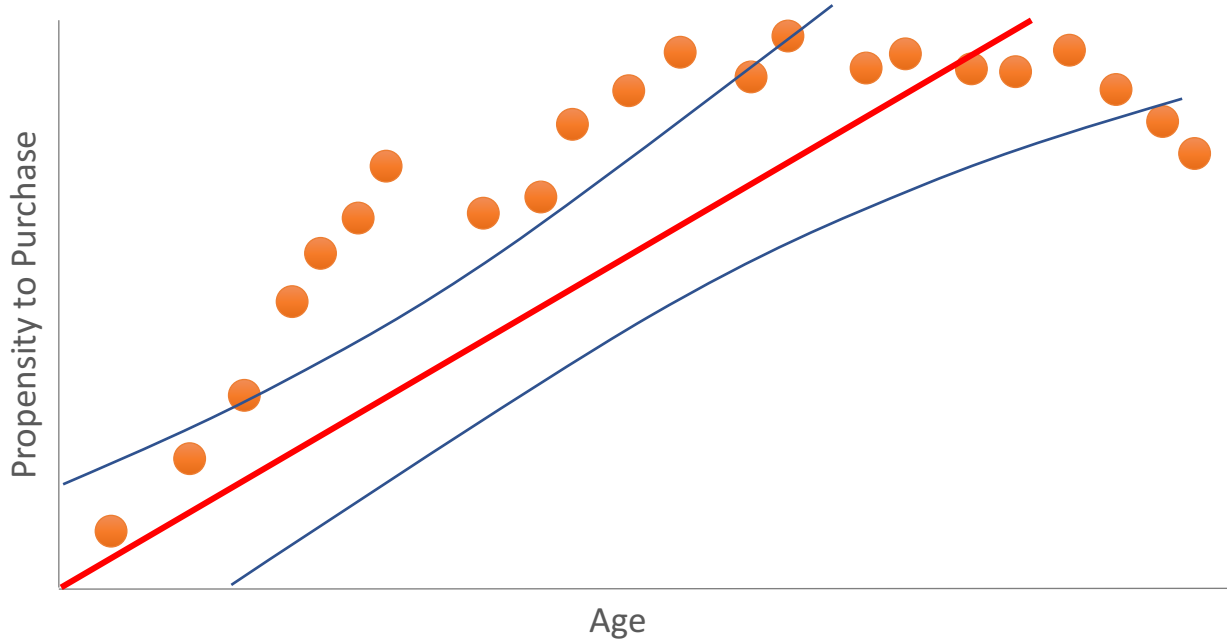
Linear Models

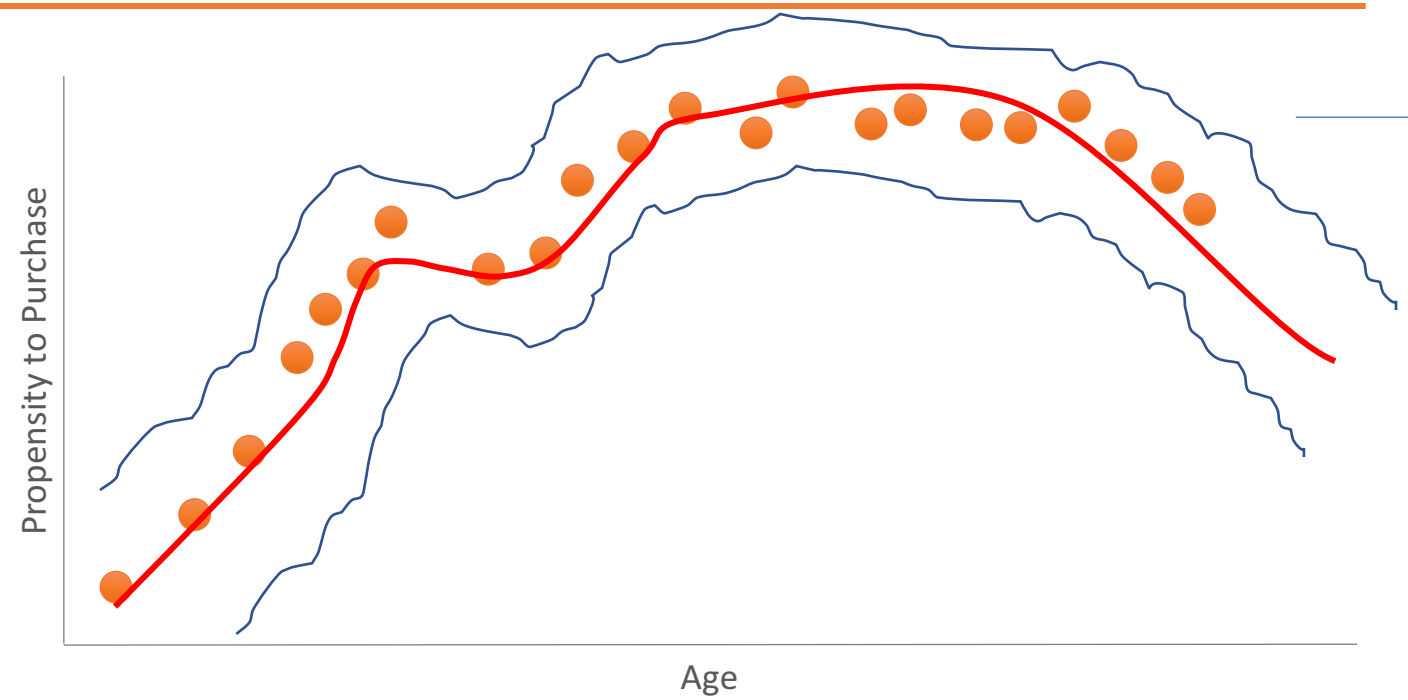
Risk is well defined …
Theoretically …
Based on **strong assumptions**.



Alpha = 0.05
Confidence Bands

Machine Learning

Risk is **empirically quantifiable** …
But it's **hard work**.



Empirically Derived
Prediction Bands

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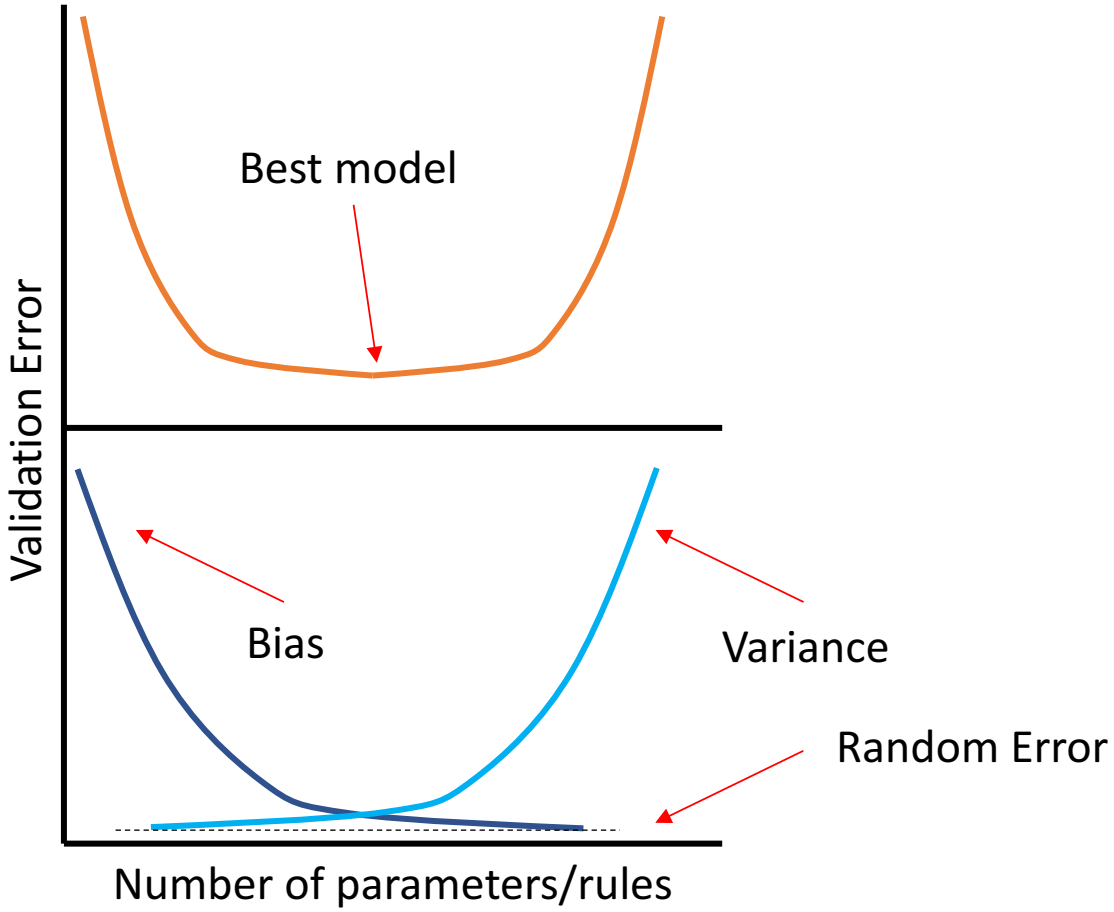
Nobody really believes that multivariate data is multivariate normal, but that data model occupies a large number of pages in every graduate textbook on multivariate statistical analysis.

-- Leo Breiman

Risk from Unwanted Bias and Prediction Variance

Total Error = Bias + Variance + Random Error =
$(\hat{f}(x) - f(x))^2$



Bias = $E[\hat{f}(x)] - f(x)$ or the error that arises from a model's inability to replicate the fundamental phenomena represented by a data set.

Variance = $(\hat{f}(x) - E[\hat{f}(x)])^2$ or the error that arises from a model's ability to produce differing predictions from the values in a new data set.

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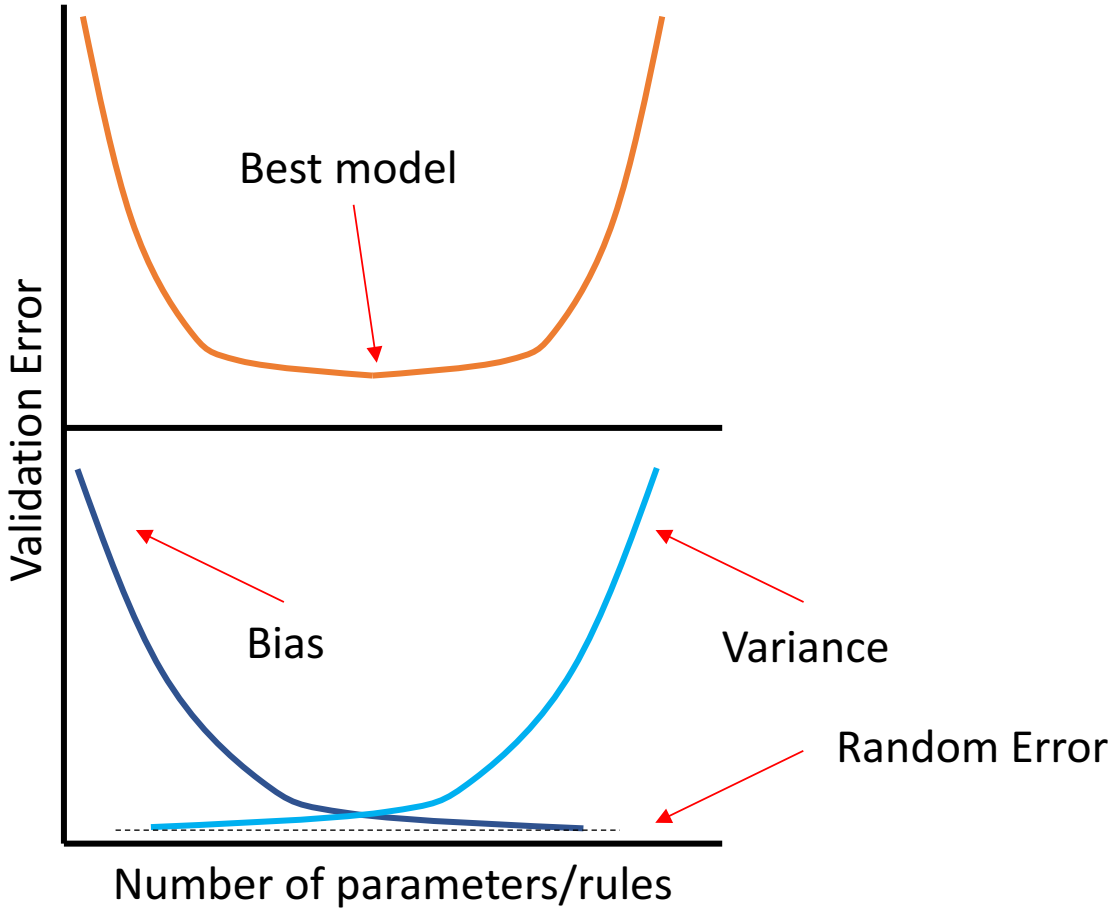
Risk from Unwanted Bias and Prediction Variance

Total Error = Bias + Variance + Random Error =

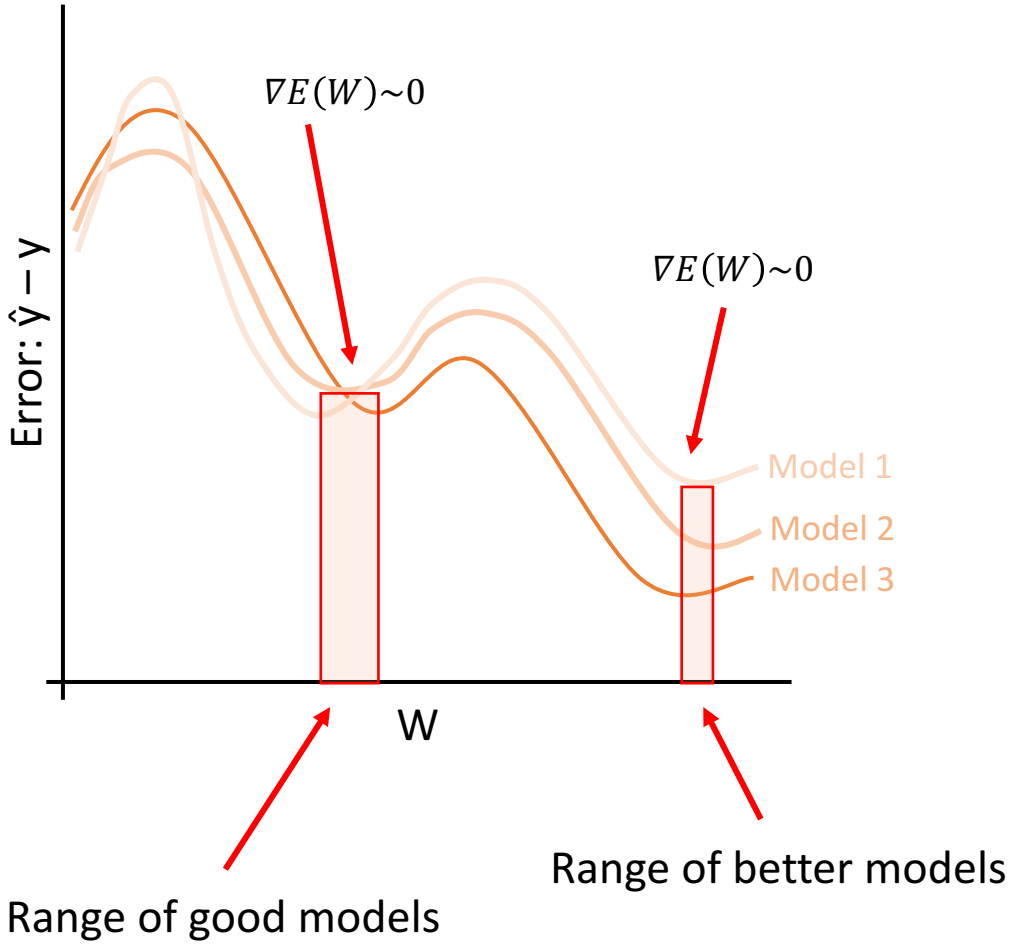
$$(\hat{f}(x) - f(x))^2$$



Risk from Unwanted Bias: Your model includes contributions from race, gender, disability status, marital status, or other unwanted latent features.

Risk from Prediction Variance: Your model is unpredictable outside of the training domain.

The Multiplicity of Good Models



Training ML models often involves solving non-convex optimization problems with multiple local minima.

Different solutions for a good ML model produce the same distribution of model outputs, *but* the actual numeric predictions produced can be slightly different.

These small differences will result in slightly different explanations. Mathematically this is ok … it's a different model after all, *but* it poses serious philosophical and regulatory problems.

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A framework for interpretability

Complexity of learned functions:
- Linear, monotonic
- Nonlinear, monotonic
- Nonlinear, non-monotonic

Scope of interpretability:
Global vs. local

Enhancing trust and understanding:
the mechanisms and results of an interpretable model should be both transparent AND dependable.

Application domain:
Model-agnostic vs. model-specific

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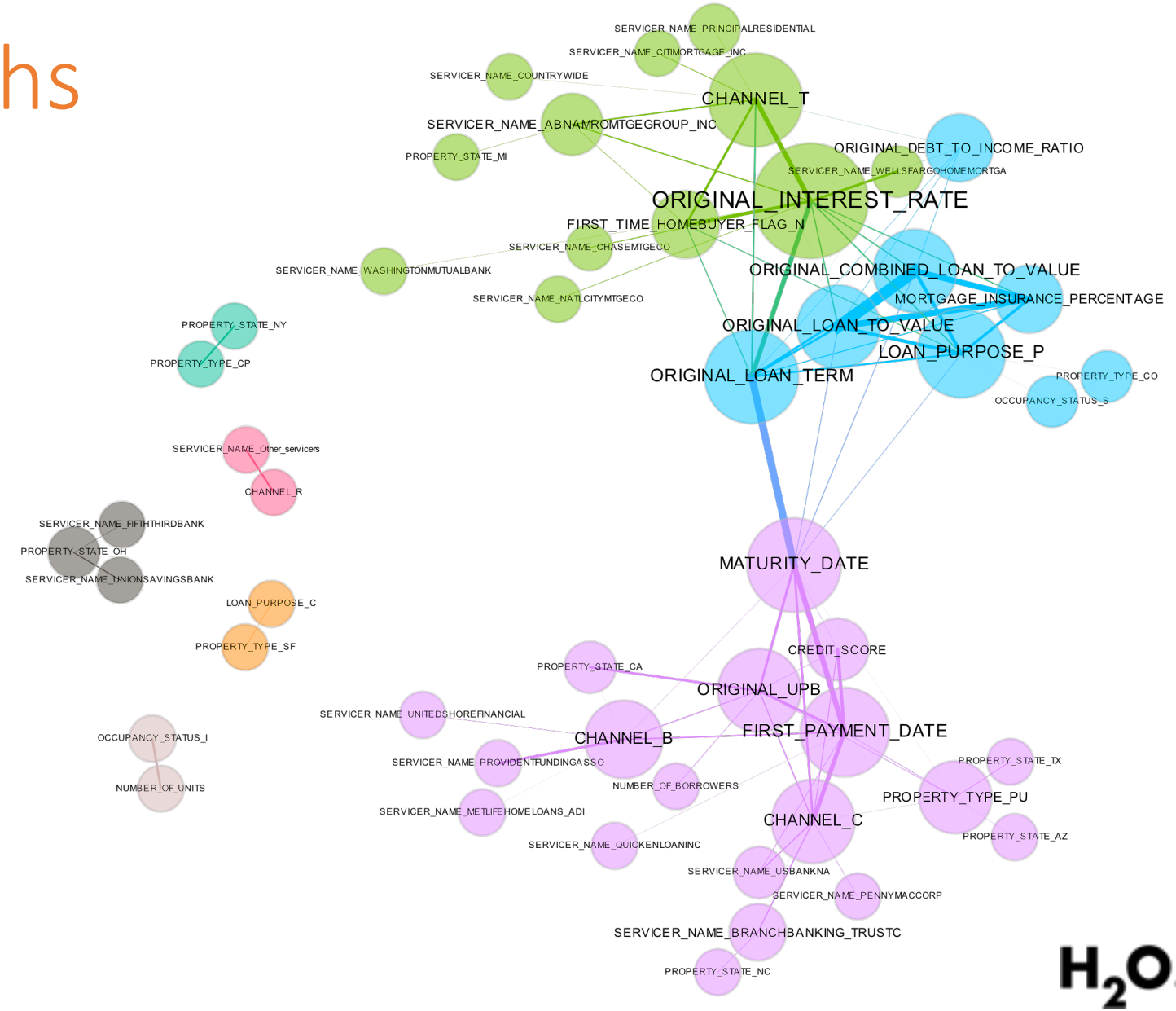
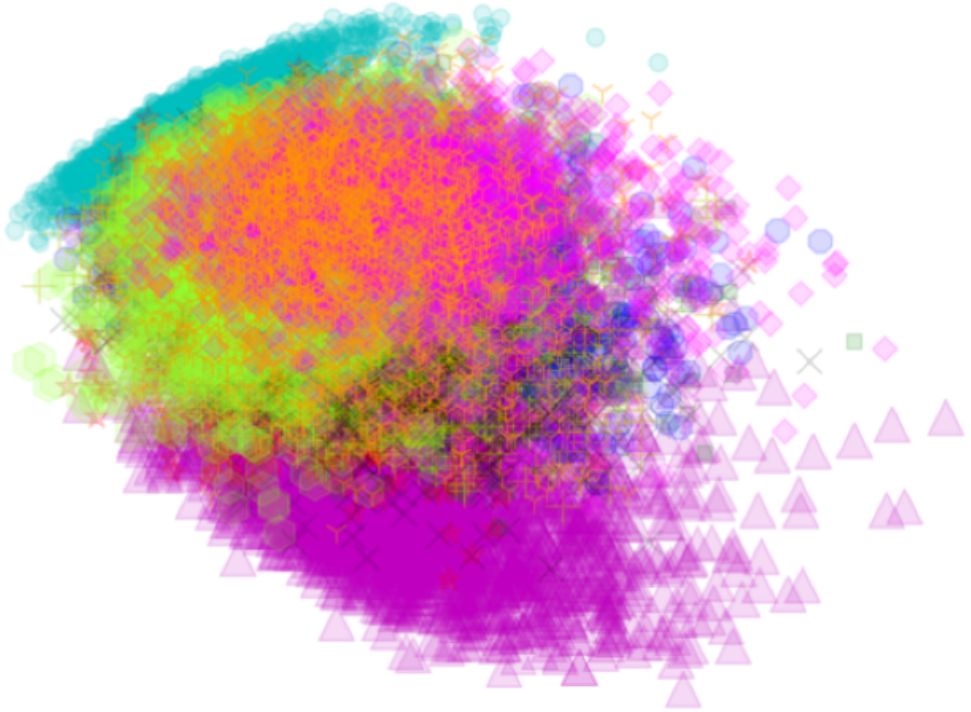
A Few of Our Favorite Things

Correlation graphs

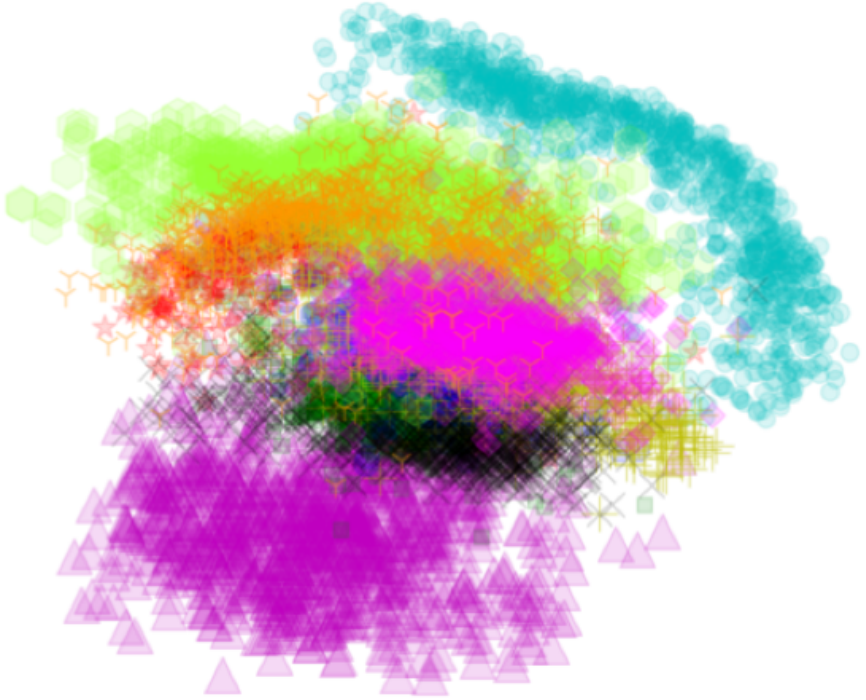
The nodes of this graph are the variables in a data set. The weights between the nodes are defined by the absolute value of their pairwise Pearson correlation.



2-D projections



784 dimensions to 2 dimensions with PCA



784 dimensions to 2 dimensions with autoencoder network

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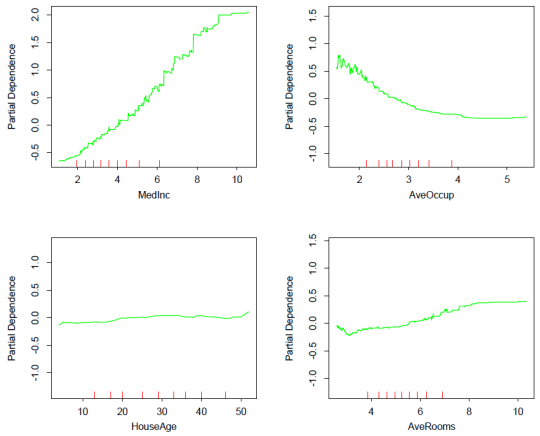
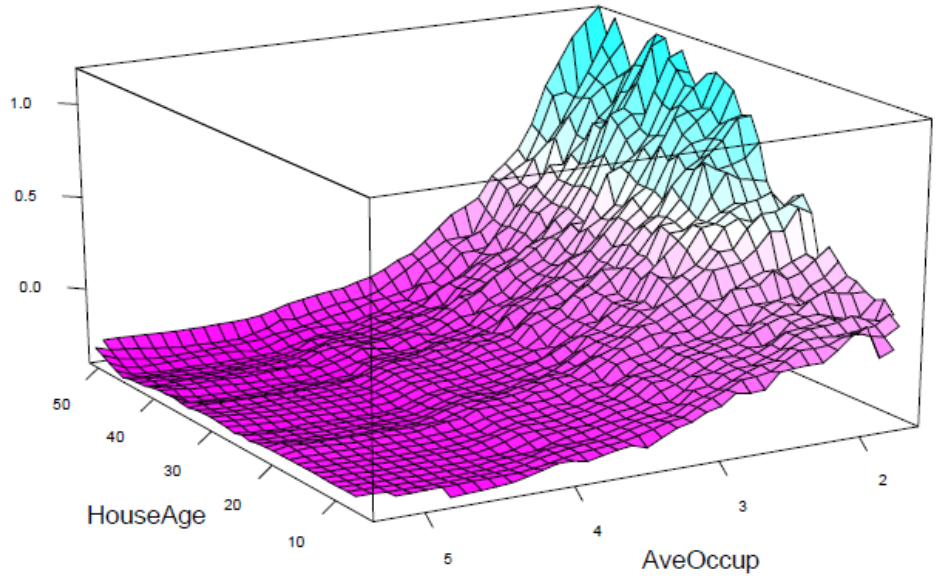
Partial dependence plots

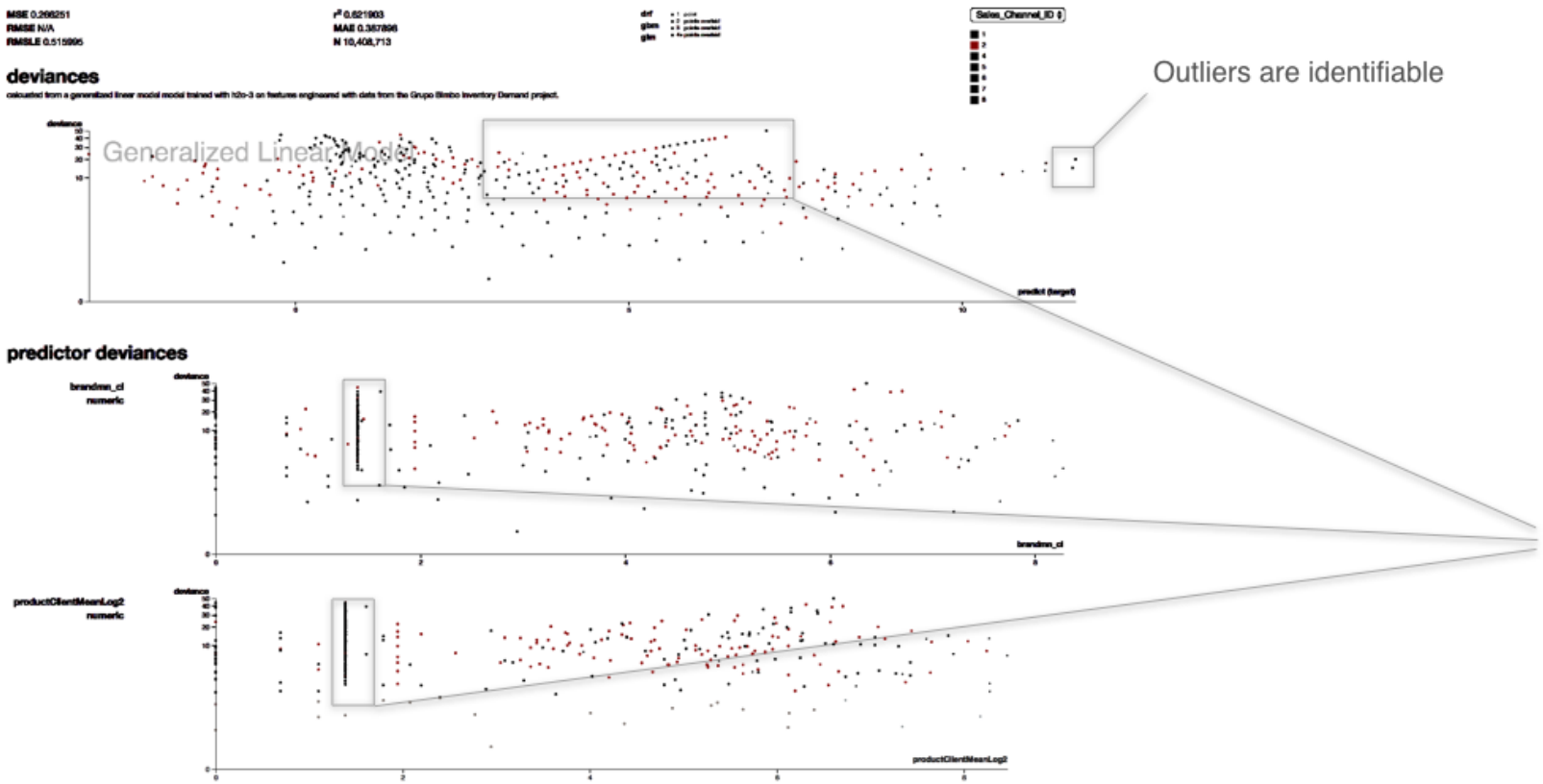




HomeValue ~ MedInc + AveOccup + HouseAge + AveRooms

Source: http://statweb.stanford.edu/~tibs/ElemStatLearn/printings/ESLII_print10.pdf

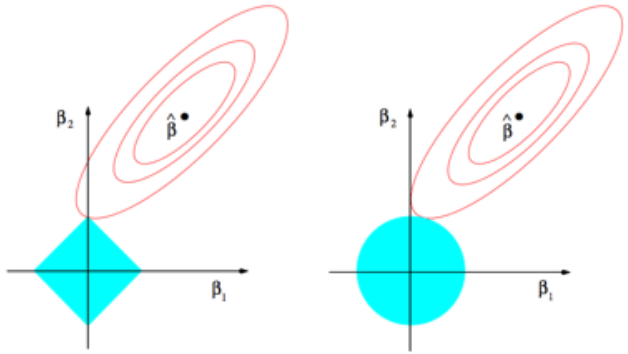
Residual analysis



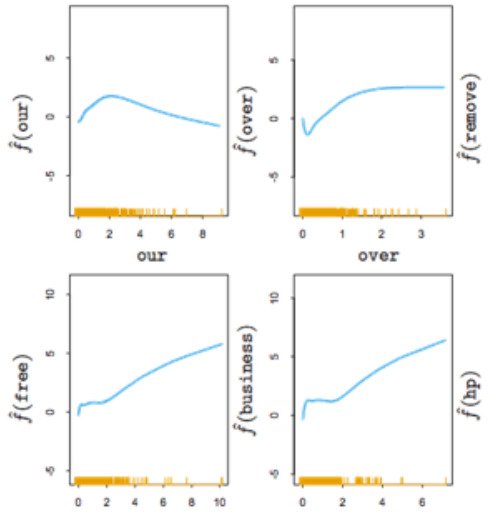
Residuals from a machine learning model should be randomly distributed

obvious patterns in residuals can indicate problems with data preparation or model specification

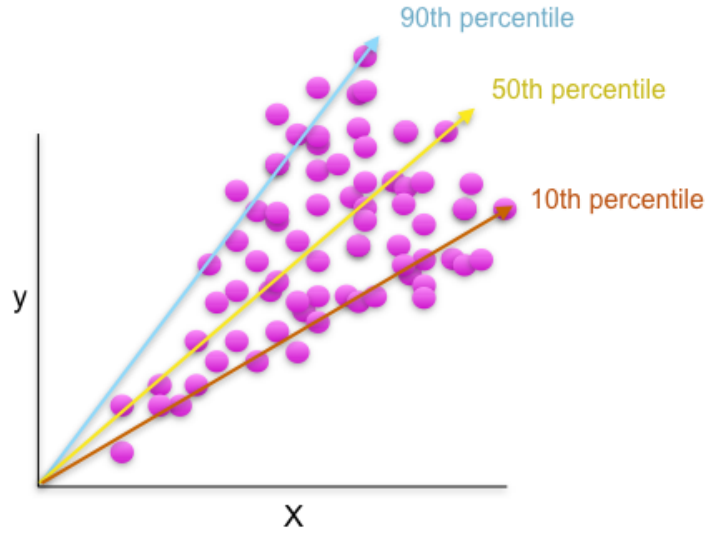
OLS regression alternatives



Penalized Regression



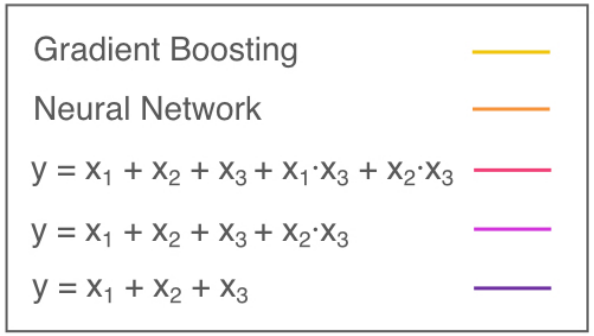
Generalized Additive Models

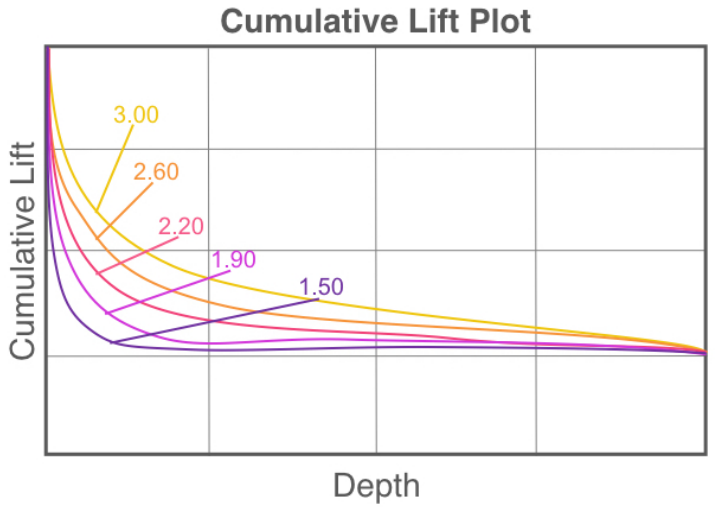


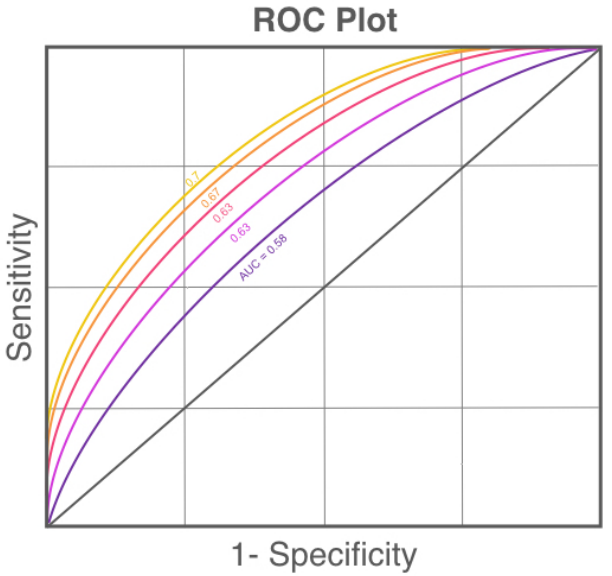
Quantile Regression

Source: http://statweb.stanford.edu/~tibs/ElemStatLearn/printings/ESLII_print10.pdf

Build toward ML model benchmarks

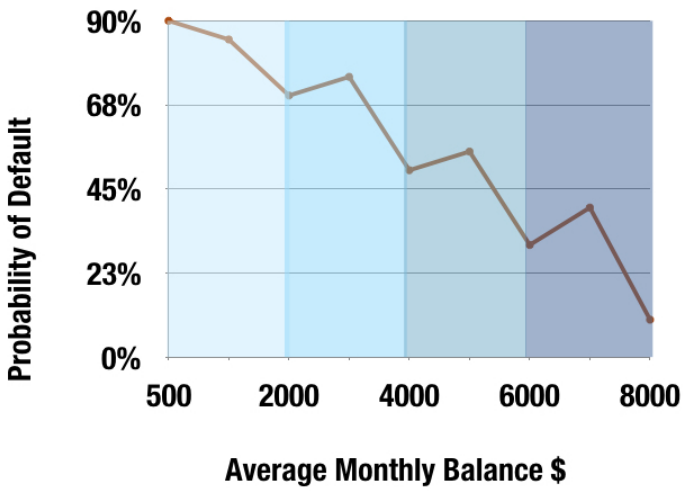




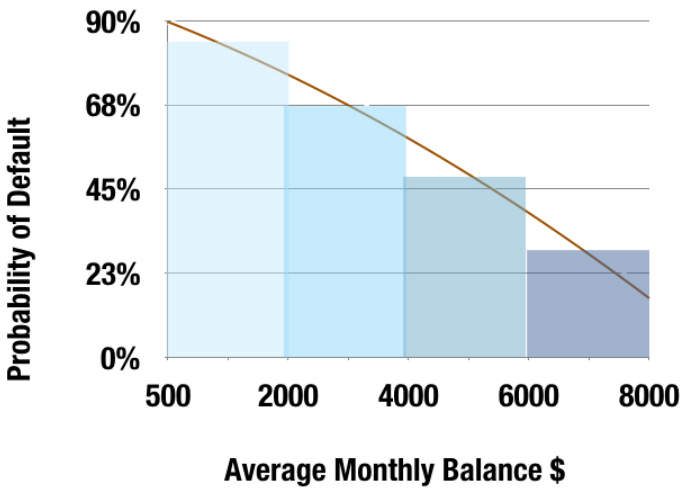


Incorporate interactions and piecewise linear components to increase the accuracy of linear models relative to machine learning models.

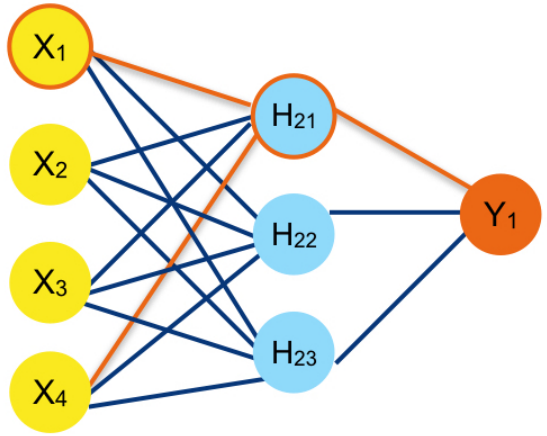
Monotonicity constraints



Average Monthly Balance is a nonnegative quantity, but is not monotonic with respect to Probability of Default.



By discretization, the Average Monthly Balance can be transformed to be monotonic with respect to the target.



When all inputs are nonnegative and monotonic with respect to the target, and model weights are constrained to be nonnegative, it's easier understand the impact of individual features and to find interactions.

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Rule-based models

IF Age: 30 <= 40 …

AND Income: 70K <= 80K …

AND Zip Code == 20009 …

AND Marital Status == SINGLE …

AND Loyalty Status == SILVER …

THEN Probability = 0.7463

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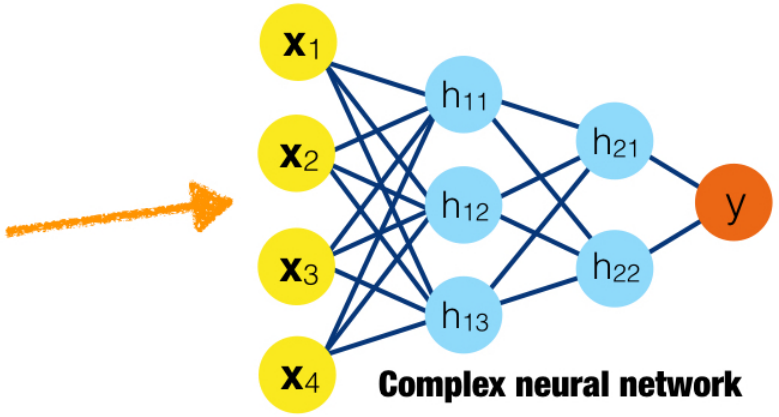
Surrogate models

BAD	CUSTOMER_DTI	LOAN_PURPOSE	CHANNEL
0	0.18	MORT	7
1	0.42	HELOC	10
0	0.11	MORT	10
0	0.21	MORT	1

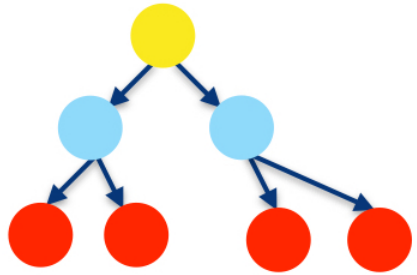
1. Train a complex machine learning model



Complex neural network

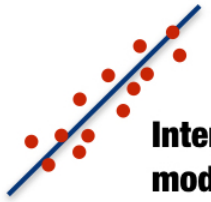
BAD	PREDICTED_BAD	CUSTOMER_DTI	LOAN_PURPOSE	CHANNEL
0	0.47	0.18	MORT	7
1	0.82	0.42	HELOC	10
0	0.18	0.11	MORT	10
0	0.12	0.21	MORT	1

2. Train an interpretable model on the original inputs and the predicted target values of the complex model



Interpretable decision tree

Or



Interpretable linear model

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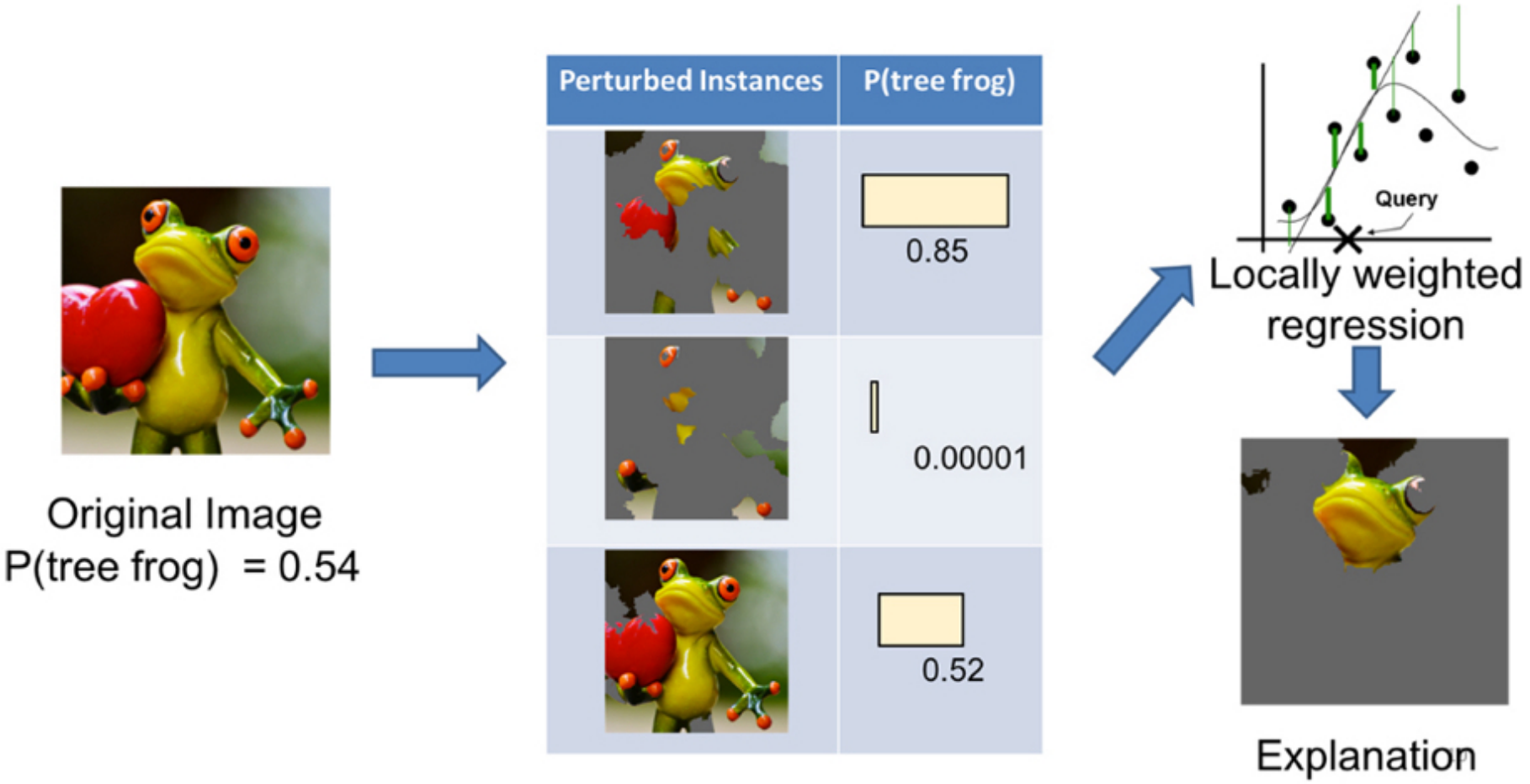
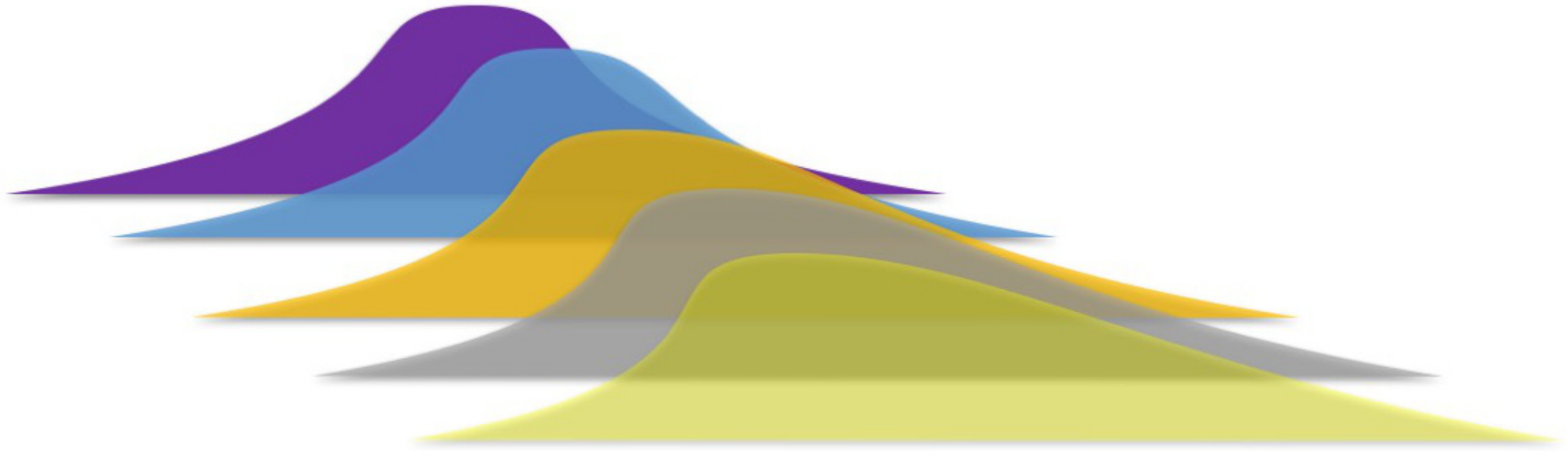
Local interpretable model-agnostic explanations



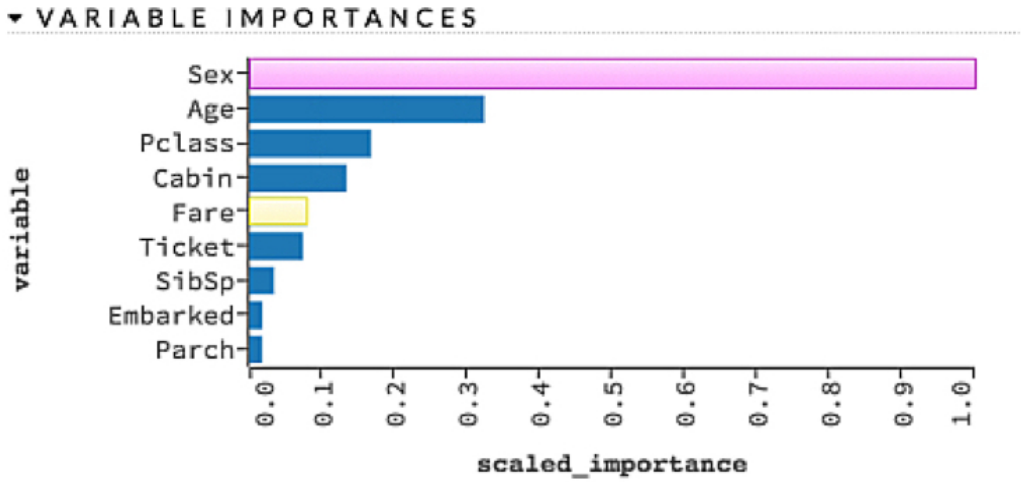
Source: https://www.oreilly.com/learning/introduction-to-local-interpretable-model-agnostic-explanations-lime

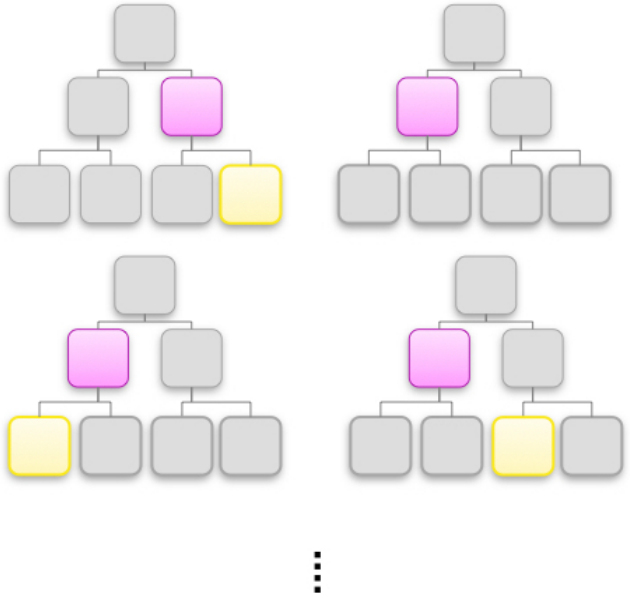
Sensitivity analysis



Data distributions shift over time. How will your model handle these shifts?

Variable importance measures





Global variable importance indicates the impact of a variable on the model for the entire training data set.

Sex	Age	…	Fare	ŷ	ŷ(-Sex)	ŷ(-Age)	…	ŷ(-Fare)
M	11	…	8.45	0.2	0.01	0.1	…	0.21
F	34	…	51.86	0.8	0.6	0.65	…	0.78
M	26	…	21.08	0.5	0.2	0.3	…	0.53
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

Local variable importance can indicate the impact of a variable for each decision a model makes – similar to reason codes.

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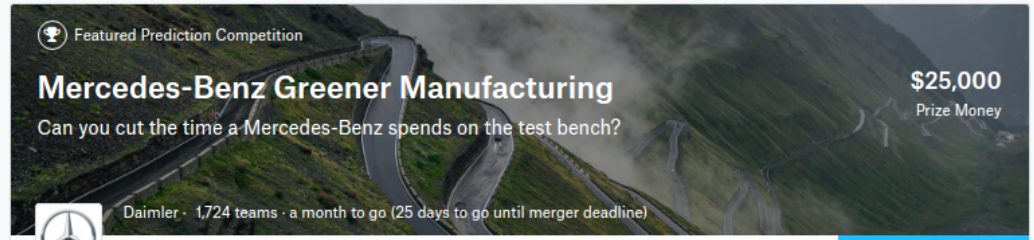
H20.ai Driverless AI



Your most recent submission

Name	Submitted	Wait time	Execution time	Score
blend.csv	just now	1 seconds	0 seconds	0.56842

Complete

Jump to your position on the leaderboard

Public Leaderboard | Private Leaderboard

This leaderboard is calculated with approximately 19% of the test data.
The final results will be based on the other 81%, so the final standings may be different.

Raw Data Refresh

In the money Gold Silver Bronze

#	△1w	Team Name	Kernel	Team Members	Score	Entries	Last
1	–	Utkarsh			0.57456	40	9h
2	▲531	plantsgo			0.57005	9	3h
3	▼1	Fred Navruzov			0.56904	23	4d
4	new	kongshuchen			0.56856	5	13h
5	▲115	Jughead			0.56844	27	5h
6	▲29	H2O.ai Driverless AI			0.56842	11	now

Your Best Entry ↑

Your submission scored 0.56842, which is an improvement of your previous score of 0.56605. Great job! Tweet this!

#	△1w	Team Name	Kernel	Team Members	Score	Entries	Last
7	▼4	happiness			0.56814	25	1d
8	▲389	Luis Moneda			0.56809	15	12h
9	–	Pan Tofelek			0.56800	35	12h
10	▼6	gotohell1			0.56790	15	16h

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0.0.1

TRAINING DATA

DATASET

default_of_credit_card_clients.csv

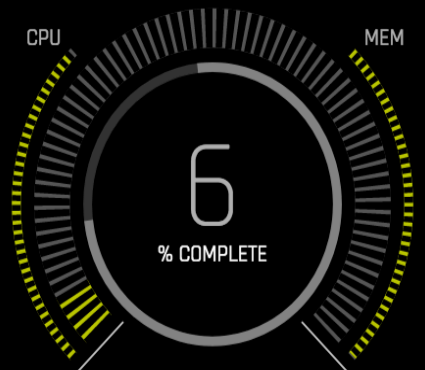
ROWS	COLUMNS	DROPPED	IGNORED
35m	24	0	0

TARGET COLUMN

default_on_payment

TYPE	MISSING	LEVELS	MEAN
float	3%	11	56.7

STATUS: RUNNING



ELAPSED 00:00:17

STOP

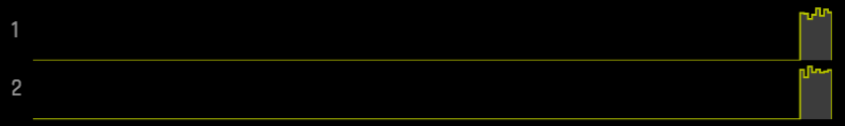
ITERATION 3 / 50

EXPERIMENT SETTINGS

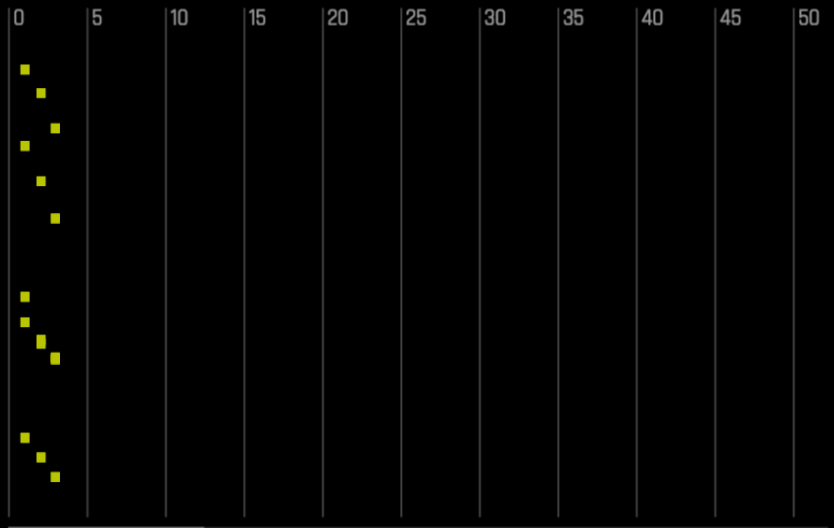
DETECT IDS

DROP DUPS.

GPU STATS



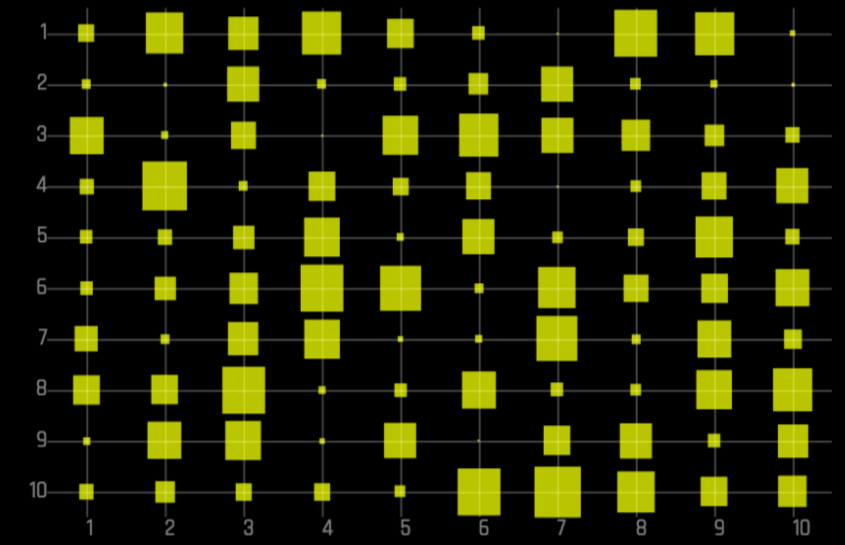
ITERATION SCORES



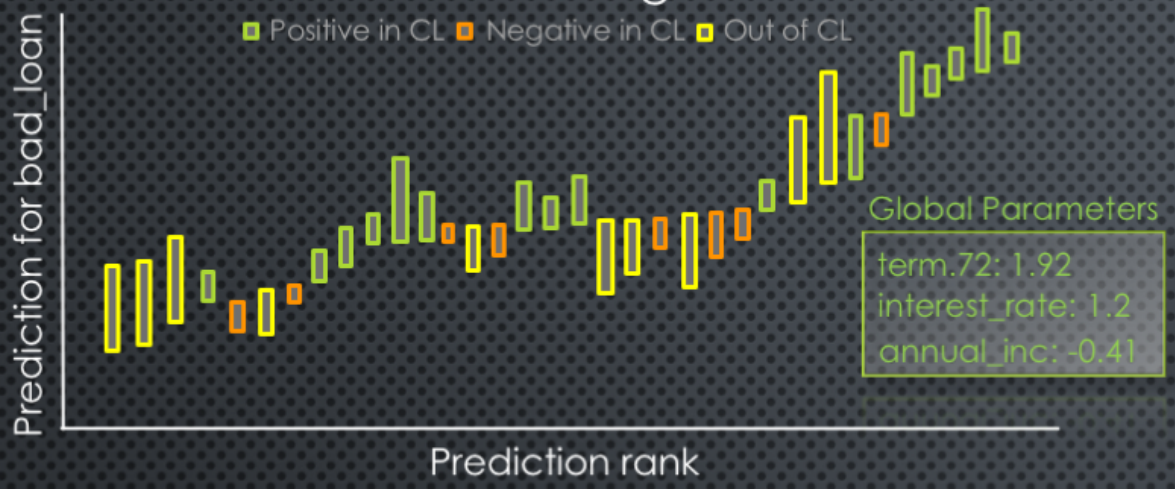
VARIABLE IMPORTANCE

PAY_4	58
PAY_3	16
LIMIT_BAL	3
BILL_AMT5	46
PAY_AMT5	62
PAY_AMT3	88
BILL_AMT2	72
ID	77
AGE	47
PAY_0	35
SEX	76
BILL_AMT3	15
EDUCATION	94
PAY_6	20

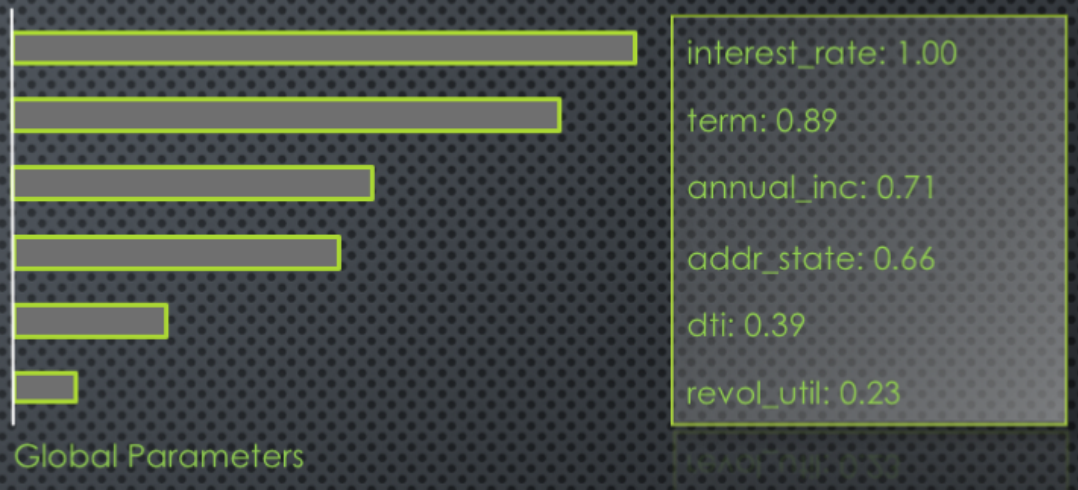
FEATURE TRANSFORMATIONS



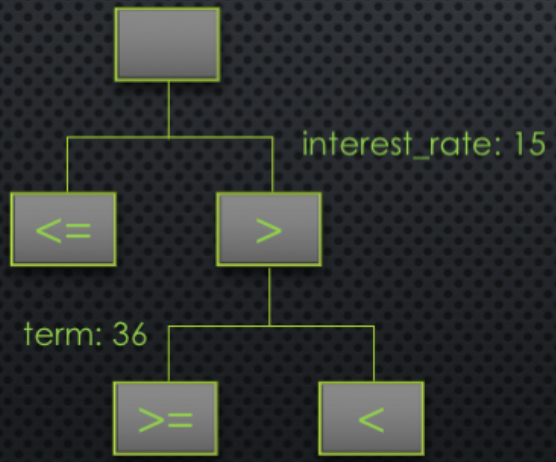
k-LIME Surrogate



Variable Importance



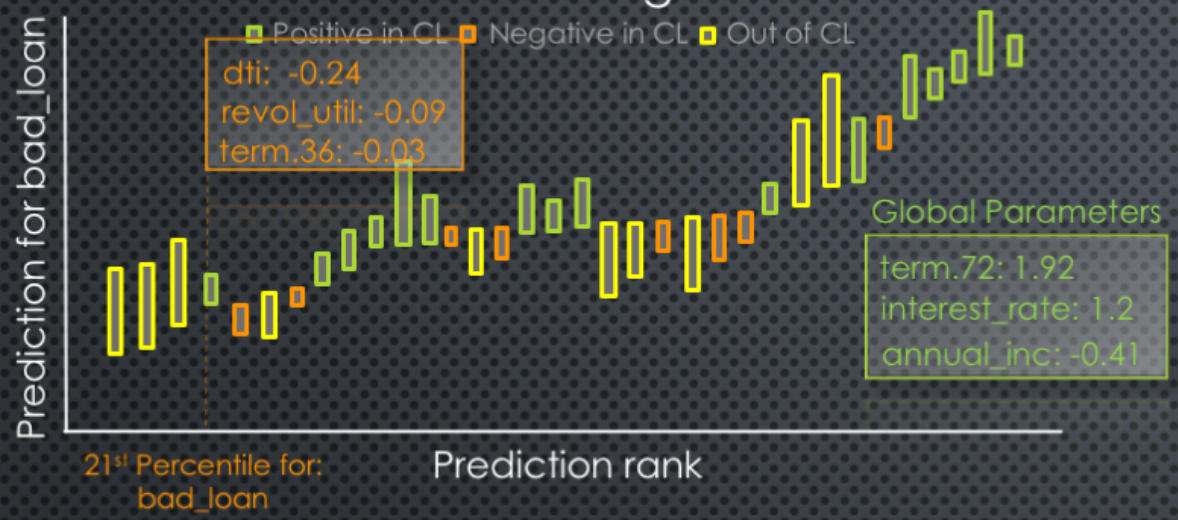
Decision Tree Surrogate



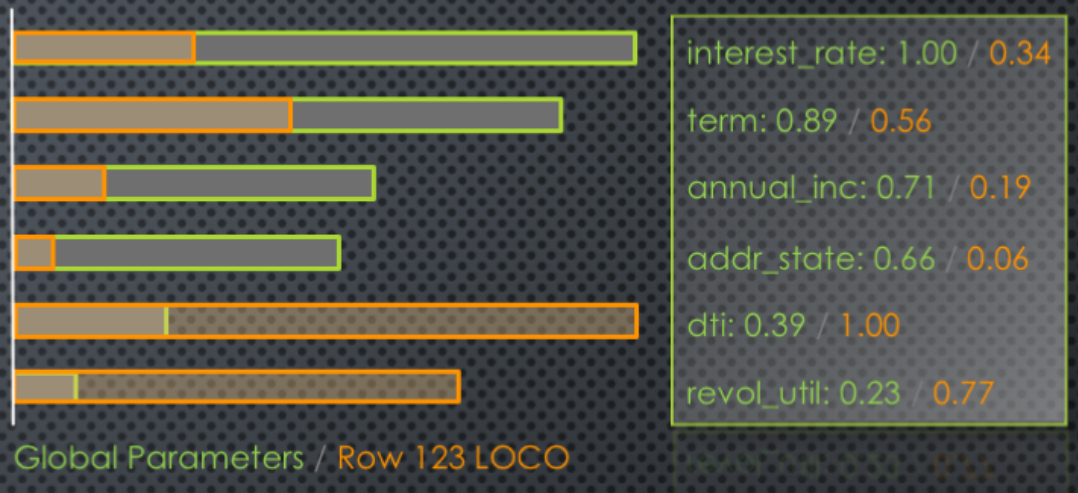
Partial Dependence

Globally, on average …
term = 72 causes a 1.92-unit **increase** in the probability of bad_loan.
A 1-unit change in interest_rate causes a 1.2-unit **increase** in the probability of bad_loan.
A 1-unit change in annual_inc causes a 0.41-unit **decrease** in the probability of bad_loan.

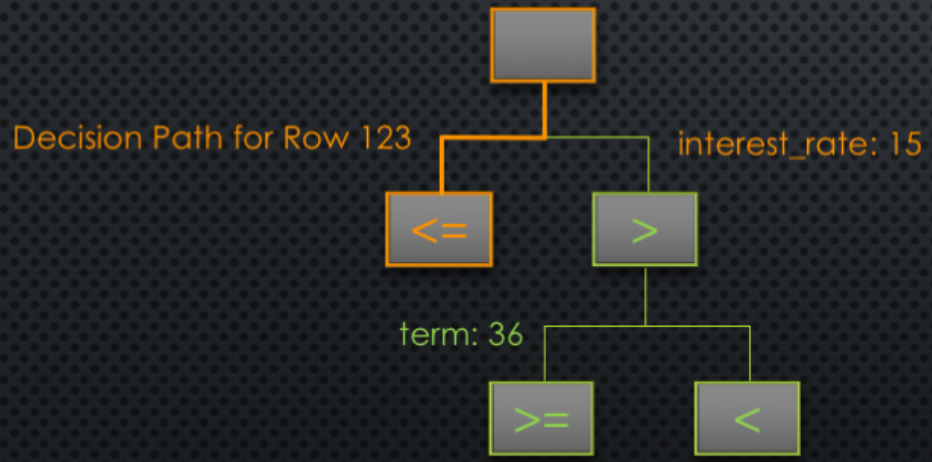
k-LIME Surrogate



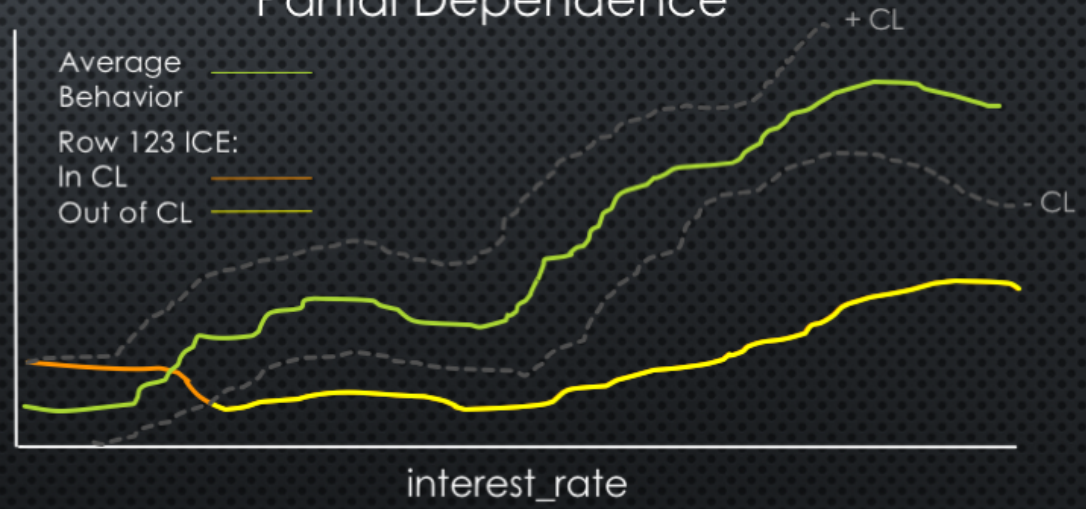
Variable Importance



Decision Tree Surrogate



Partial Dependence



Globally, on average …
term = 72 causes a 1.92-unit **increase** in the probability of bad_loan.
A 1-unit change in interest_rate causes a 1.2-unit **increase** in the probability of bad_loan.
A 1-unit change in annual_inc causes a 0.41-unit **decrease** in the probability of bad_loan.

Locally, for row 123 …
dti = 2.0 causes a 0.24-unit **decrease** in the probability of bad_loan.
revol_util = 50.0 causes a 0.09-unit **decrease** in the probability of bad_loan.
term = 36 causes a 0.03-unit **decrease** in the probability of bad_loan.

Questions?