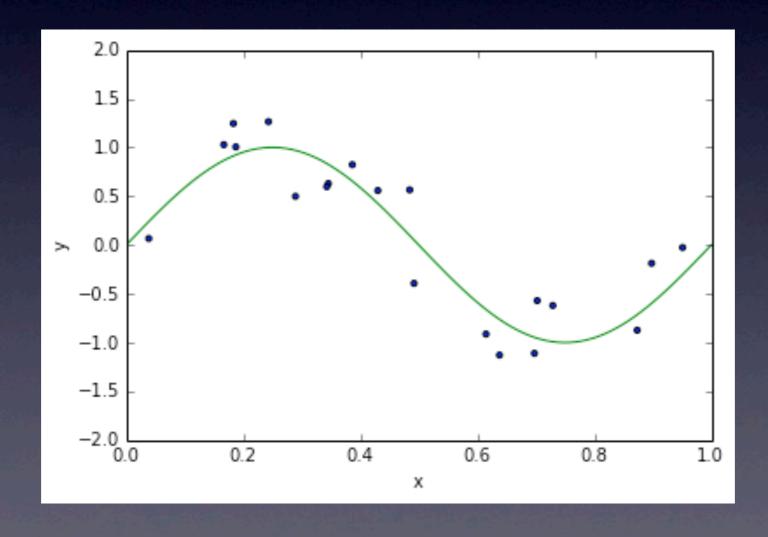
Machine Learning Introduction

Kristen Menou

Example Data

20 datapoints for sinusoid + gaussian noise: y=f(x)



Definitions/Conventions

- Unknown function z=f(x,y) (including noise)
- Function is sampled at various data points: (x1,y1) = z1, (x2,y2)=z2, (x3,y3)=z3, etc...
- x, y are called <u>features</u> (aka <u>variables</u>)
- z is called the <u>response</u> (aka <u>target</u>, <u>label</u>)
- data points #1, 2, 3, etc... are called <u>samples</u>
 (aka <u>observations</u>)

What is ML?

"Standard Programming"



Definitions/Conventions

- Unsupervised learning: categorize/characterize/ find trends in arbitrary dataset (e.g.: clustering in x,y plane, in the absence of z)
- Supervised learning: predict after learning from a set of example datapoints: z=f(x,y)
- Regression: supervised learning with continuous, ordered response (e.g. 0-1000)
- Classification: supervised learning with categorical response (e.g. yes/no, black/white)

A variety of algorithms

Supervised Regression

- Simple and multiple linear regression
- Decision tree, random forest
- Artificial Neural networks
- Nearest neighbor methods (e.g., k-NN or k-Nearest Neighbors)
- •

Supervised Two-class & Multi-class Classification

- Logistic regression and multinomial regression
- Artificial Neural networks
- Decision tree, random forest
- SVM (support vector machine)
- Bayesian classifiers (e.g., Naive Bayes)
- Nearest neighbor methods (e.g., k-NN or k-Nearest Neighbors)
- •

Unsupervised

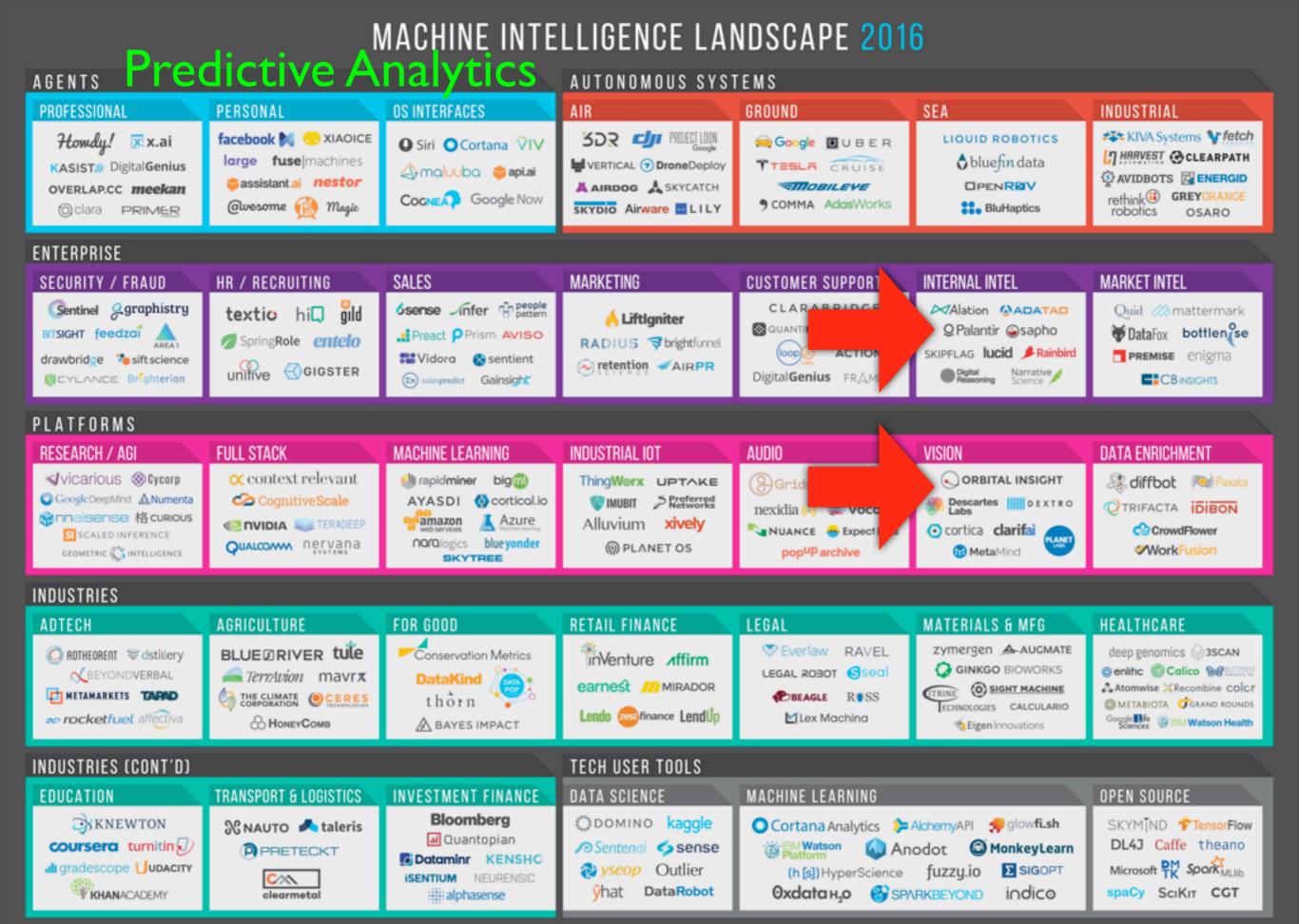
- K-means clustering
- PCA (principal component analysis)
- •

ML project: general steps

- Data selection and pre-processing
- Data splitting (cross-validation)
- Feature selection (remove) and feature engineering (add)
- Model selection & optimization
- Deployment/Prediction phase

General Workshop Goals

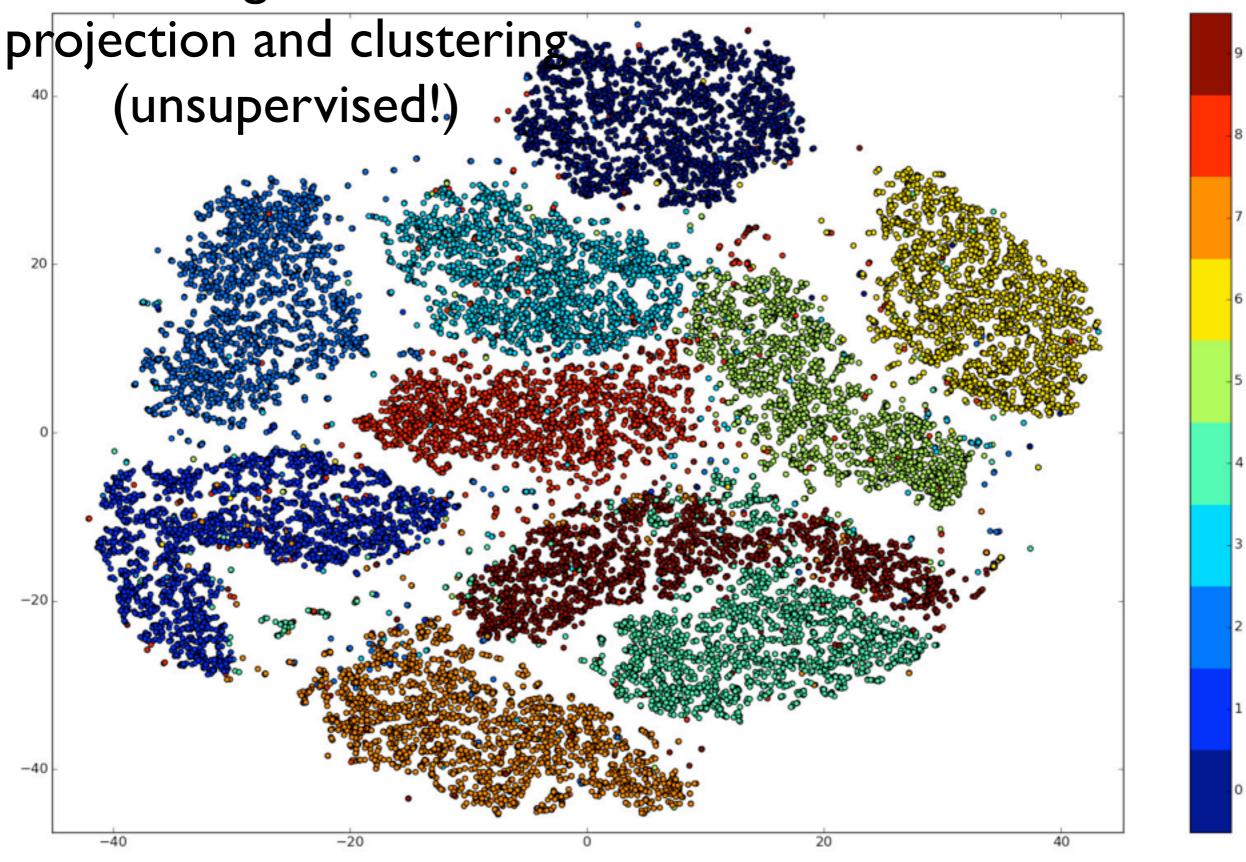
- Learn about various steps in a ML project
- Learn about various algorithms available
- Use scikit-learn platform
- Practice!
- Solve new science problems!?



State-of-the-Art

MNIST data: hand-written digits (10-class classification)

t-SNE algorithm: 2D



Deep Learning

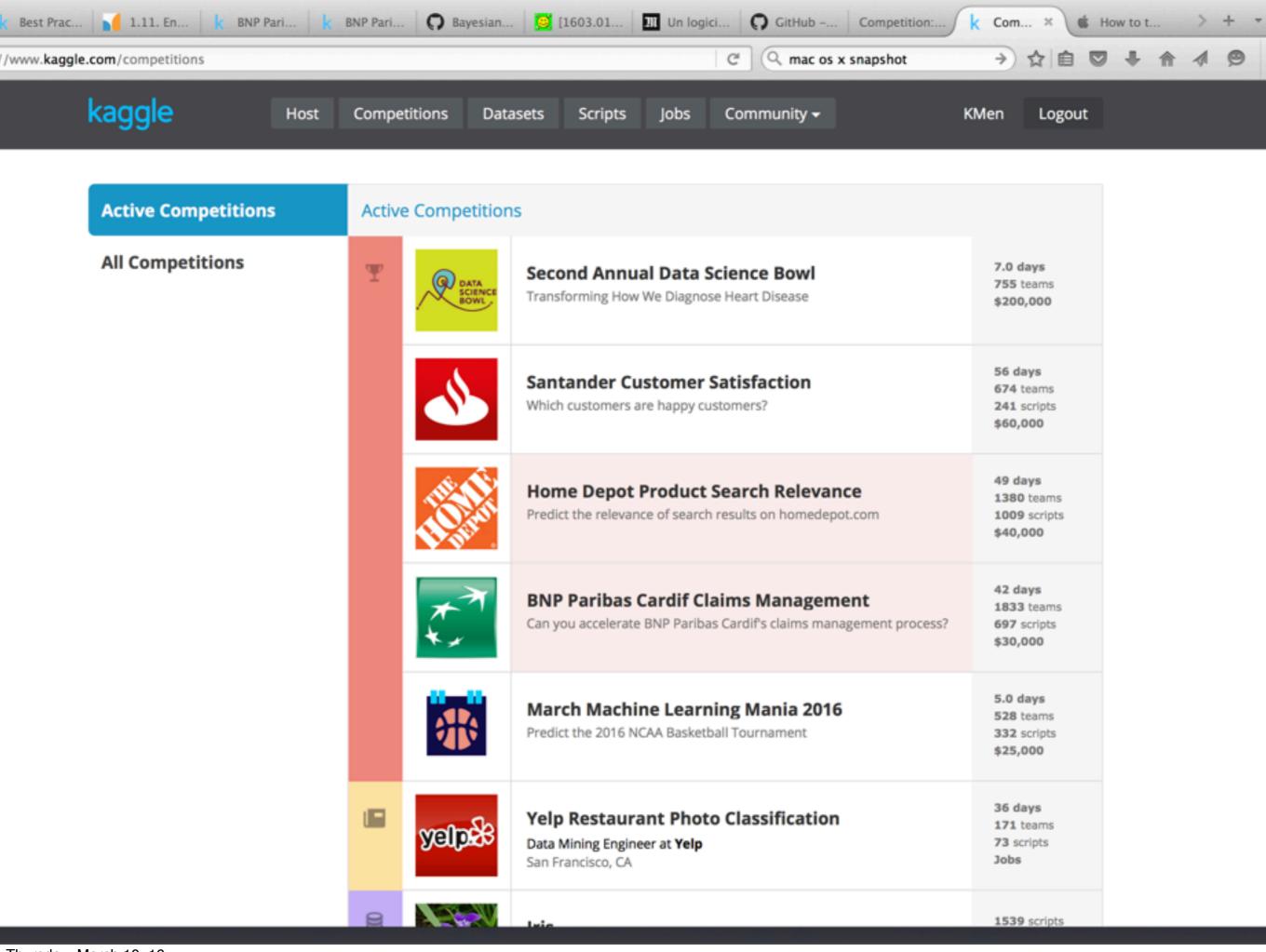


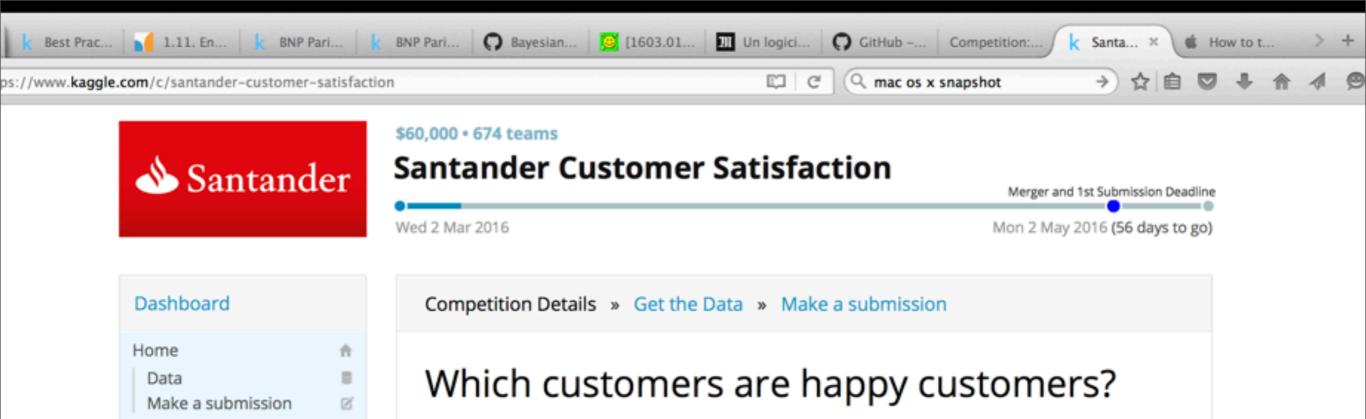
ML in practice

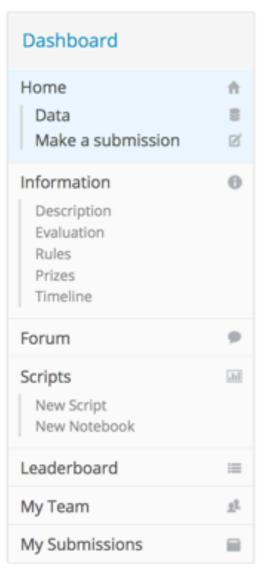
- It is unclear what constitutes the best ML solution on a given problem
- Data science competitions provide useful comparisons (+ near-optimal solutions)
- Competition & collaboration both help

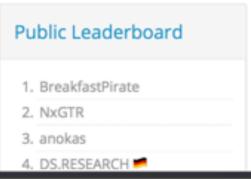
Kaggle: ML training camp

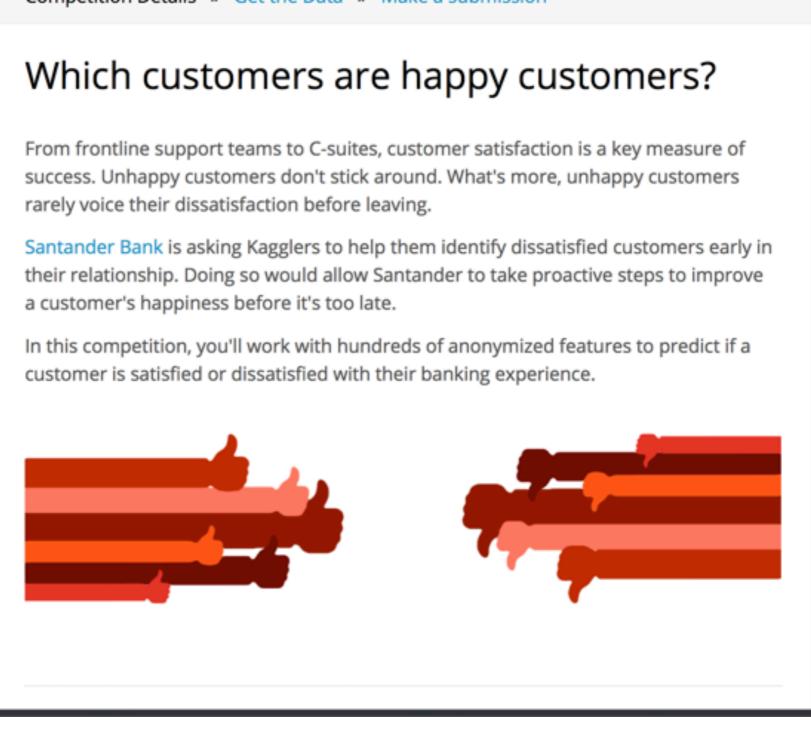
- Dataset & ML Competition Host
- Competitions: company provides data, crowd builds ML models, predict on "unseen/unlabeled" test data, best predictive model wins \$\$\$
- Company gets crowd-sourced, near-optimal ML solution for their specific data science problem
- ~500,000 kagglers, typically ~500-3000 participate in a given competition
- Key issues: feature engineering, overfitting, ML algorithms (choice + optimization)











Merger and 1st Submission Deadline



\$60,000 • 674 teams

Santander Customer Satisfaction

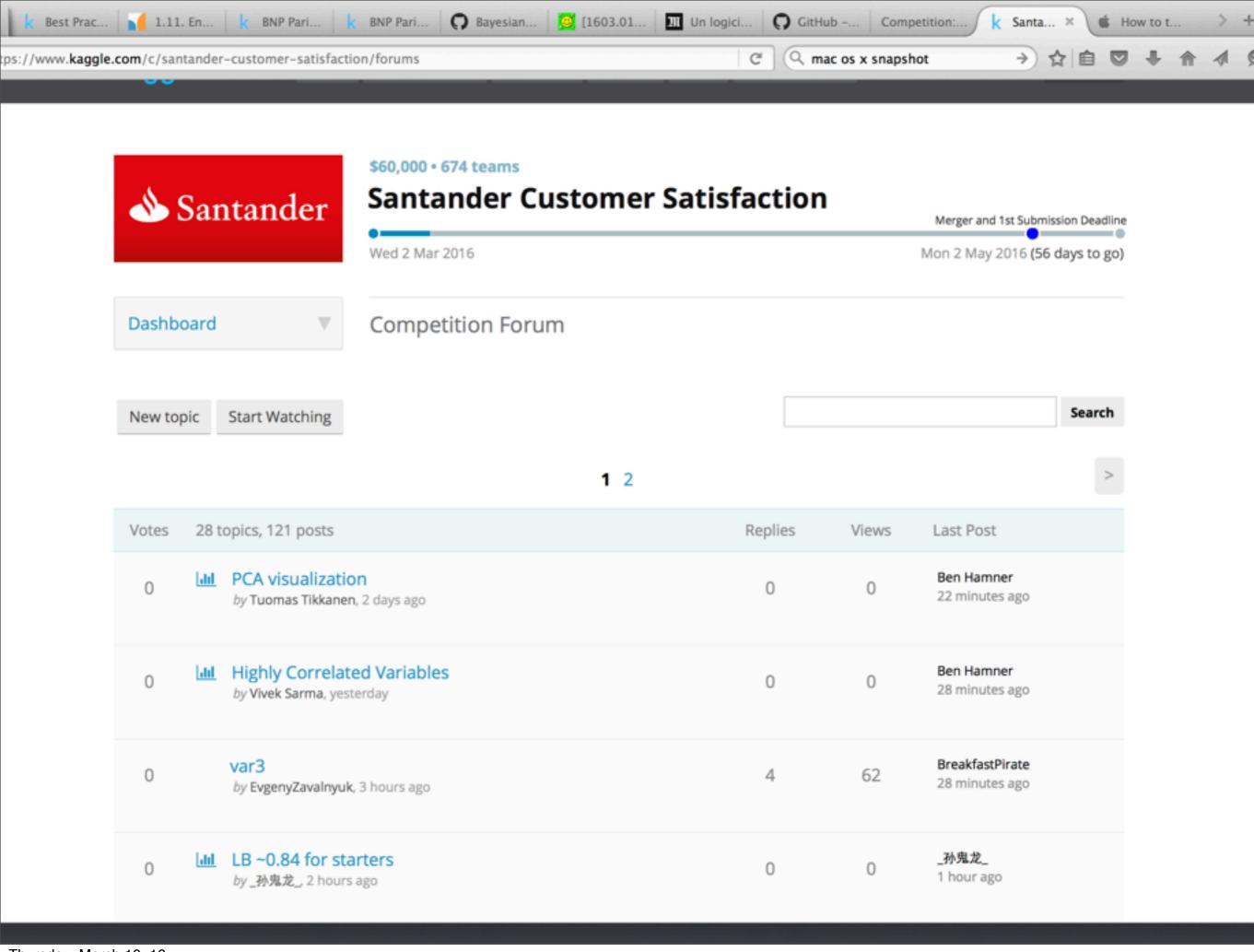
Wed 2 Mar 2016 Mon 2 May 2016 (56 days to go)

Dashboard

Public Leaderboard - Santander Customer Satisfaction

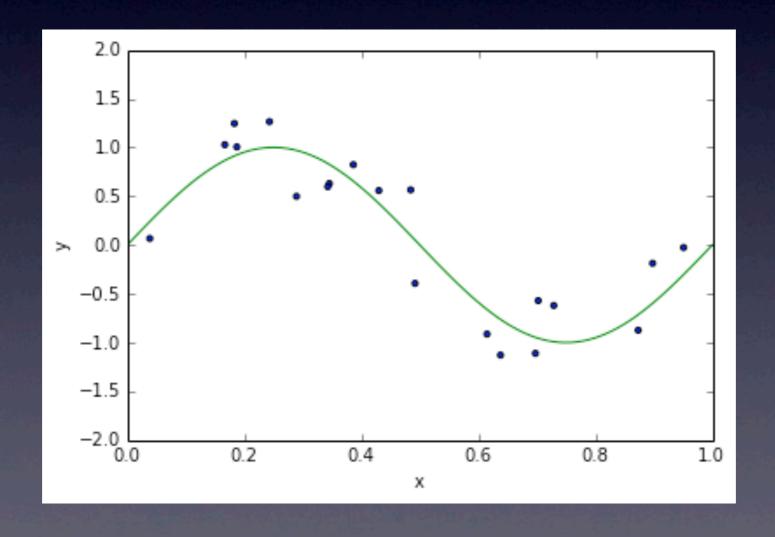
This leaderboard is calculated on approximately 50% of the test data. The final results will be based on the other 50%, so the final standings may be different. See someone using multiple accounts? Let us know.

# Δ1d Team Name ◆ In the money Score Entries Last Submission Score Entries Last Submission	n UTC (Best – Last Submission)
1 — BreakfastPirate * 0.841667 20 Mon, 07 Mar 2	2016 19:25:16 (-2.2d)
2 — NxGTR * 0.841416 17 Mon, 07 Mar 2	2016 06:32:43 (-3.2d)
3 — anokas * 0.841367 21 Mon, 07 Mar 2	2016 21:45:07 (-45.7h)
4 ↑1 DS.RESEARCH ► 0.841221 25 Mon, 07 Mar 2	2016 06:01:14 (-0.3h)
5 11 Babar16 0.841218 8 Sun, 06 Mar 20	016 21:36:32
6 — Dimitris Leventis 0.841136 25 Mon, 07 Mar 2	2016 11:38:55 (-3.1d)
7 — carl 0.841116 14 Sun, 06 Mar 20	016 21:38:37 (-24h)
8 — Florian <u>0.841112</u> 7 Fri, 04 Mar 201	16 07:07:45
9 — Kim Quy 0.841085 6 Sun, 06 Mar 20	016 09:29:59
10 — Robert Martin 0.841060 30 Mon, 07 Mar 2	2016 21:28:55 (-0.1h)
11 †400 YaronBlinder 0.840953 4 Mon, 07 Mar 2	2016 19:56:11



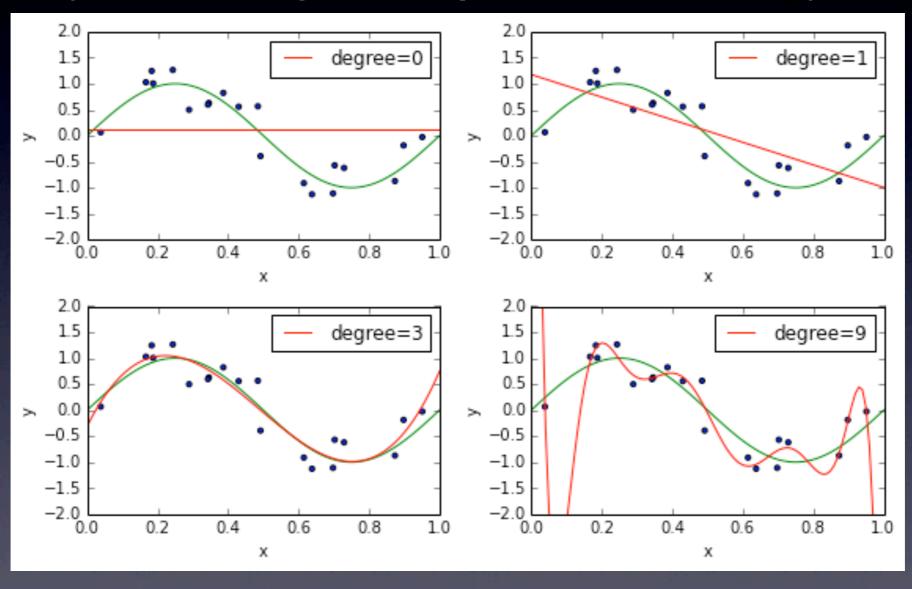
Synthetic Data

Generate 20 samples from sinusoid + gaussian noise: y=f(x)



Fitting choices

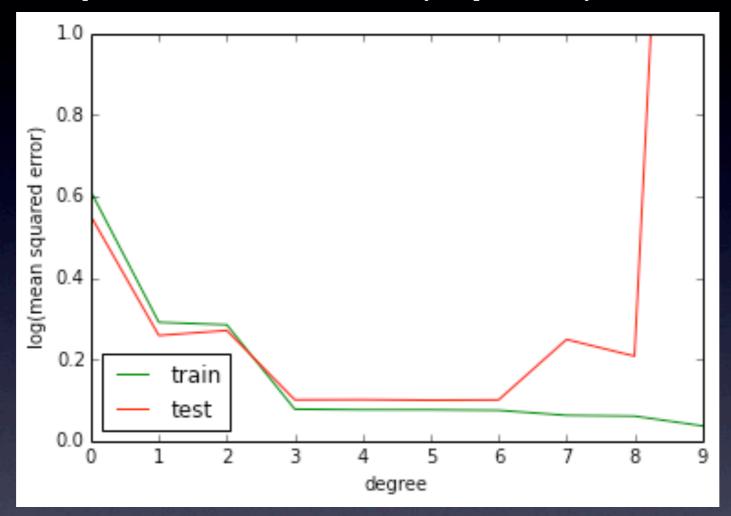
Best fit polynomials of various degrees (minimizing the squared residuals)



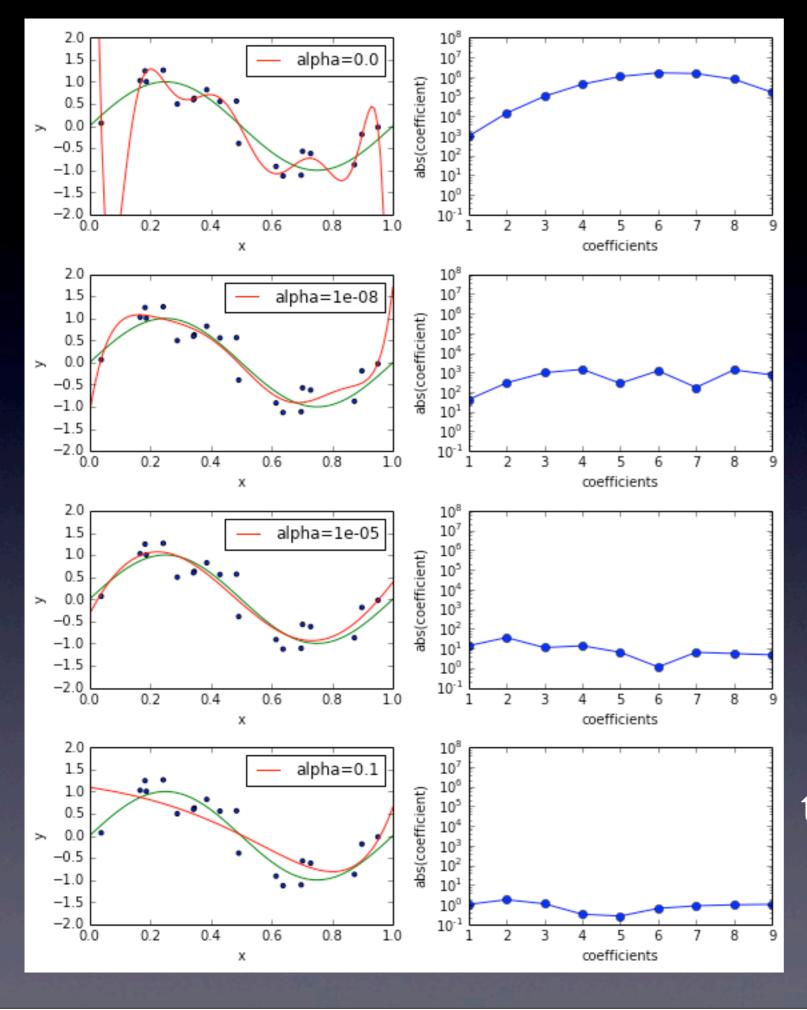
Good?

Fits the noise? "Overfitting"

Train-Test Split Split data points in train (say 2/3) and test (1/3)



Fit/Learn/Train on train set, predict on test set (mean squared error). Best model will "generalize" best on the test data (rather than "fitting the noise" in the train data)

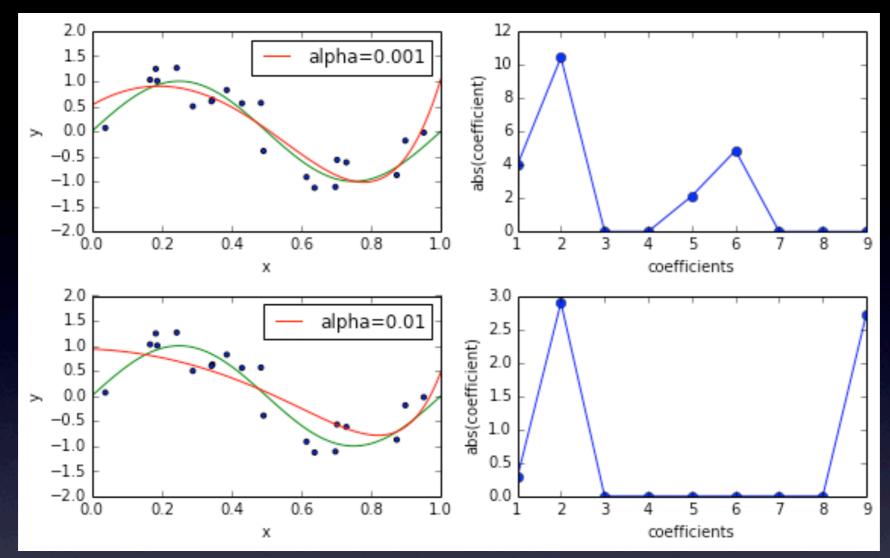


Strategy I: limit complexity

Strategy 2: regularization.

Damp coefficients of polynomial fit.

Adjust free parameter with train/test validation.



Sparse regularization: zero-out coefficients preferentially (only 3-4 non-zero).

Again train/test validation required for model evaluation.

A kind of automated feature selection!

Topics for Day-I Workshop

- Scikit-Learn
- Overfitting
- K-NN/Linear Regression
- Cross-Validation
- Plan long-term ML projects