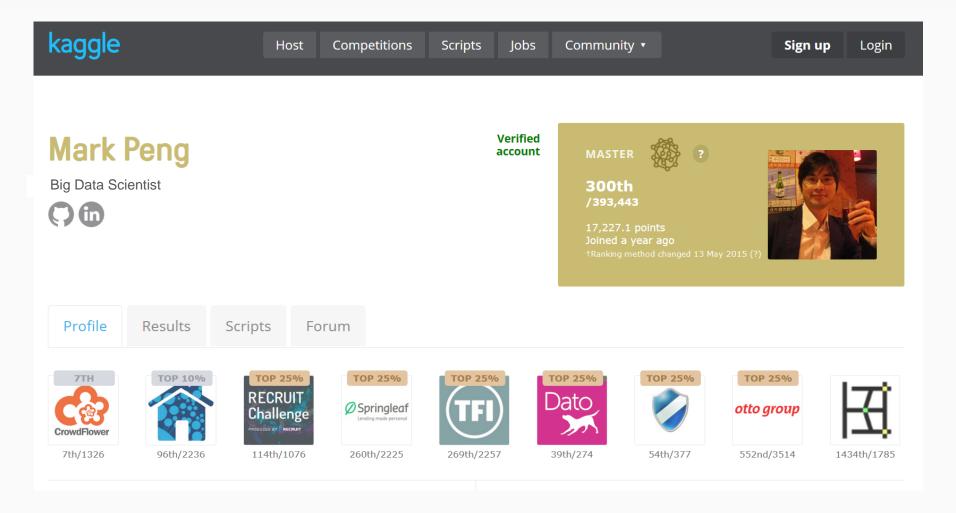
# General Tips for participating kaggle Competitions

Mark Peng 2015.12.16 @ Spark Taiwan User Group



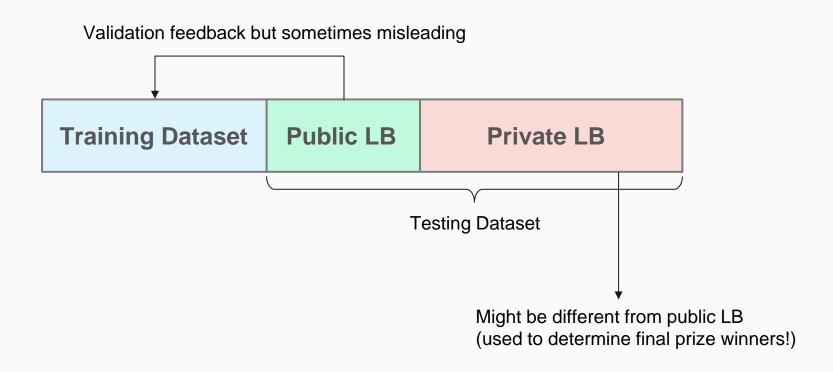
## Kaggle Profile (Master Tier)



#### Things I Want to Share

- Quick overview to Kaggle rules
- Why cross-validation matters
- Mostly used ML models
- Feature engineering methods
- Ensemble learning
- Team up
- Recommended books, MOOCs and resources

#### Kaggle Competition Dataset and Rules



#### How to become a Kaggle Master

- To achieve Master tier, you must fulfill 2 criteria
  - Consistency: at least 2 Top 10% finishes in public competitions
  - Excellence: at least 1 of those finishes in the top 10 positions
- Note that not all competitions count toward earning Master tier!

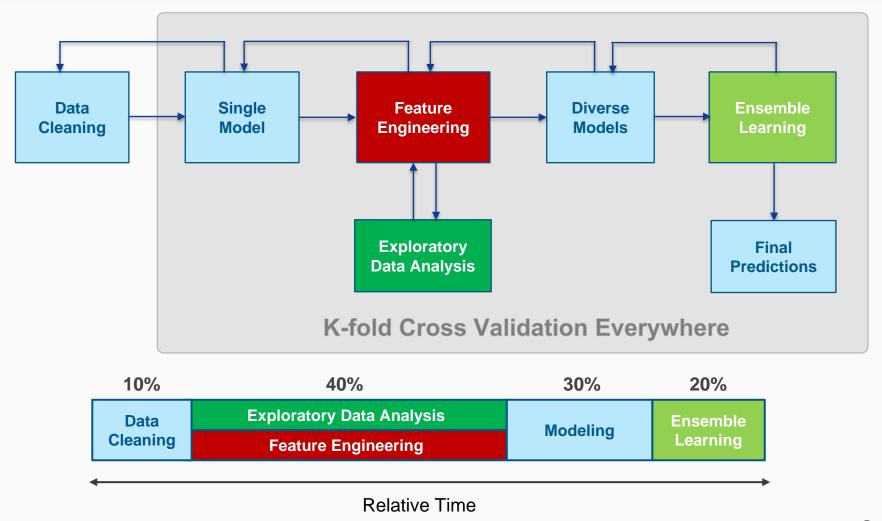
Started: 7:29 pm, Monday 9 November 2015 UTC

Ends: 11:59 pm, Monday 8 February 2016 UTC (91 total days)

Points: this competition awards standard ranking points

Tiers: this competition counts towards tiers

#### Recommended Data Science Process (IMHO)

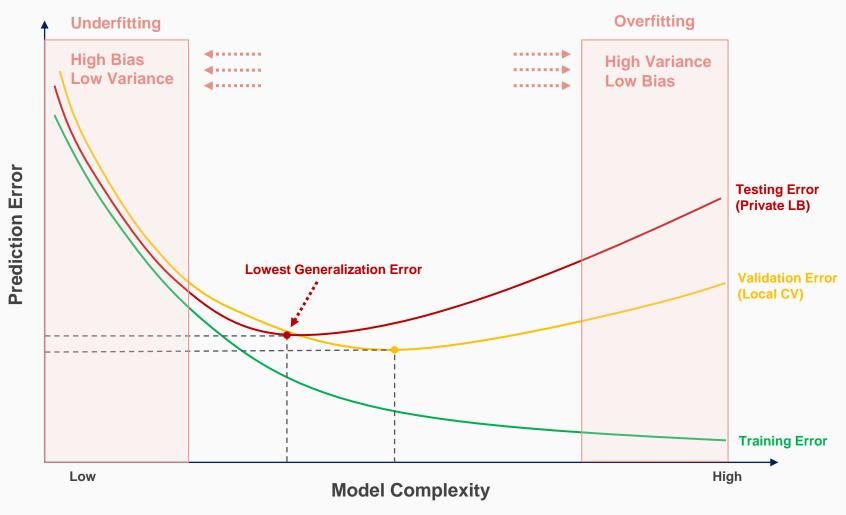


# **Cross Validation**

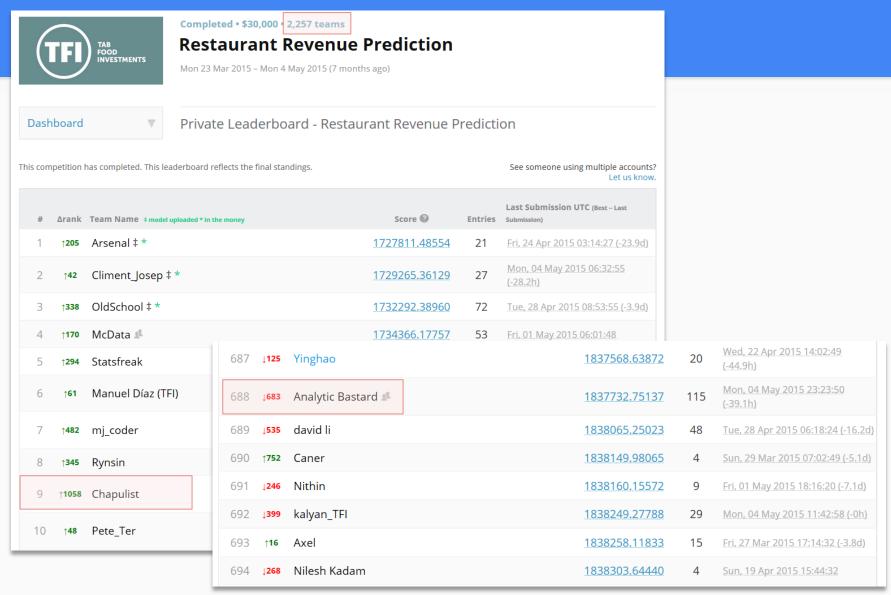
The key to avoid overfitting

## **Underfitting and Overfitting**

We want to find a model with lowest generalization error (hopefully)

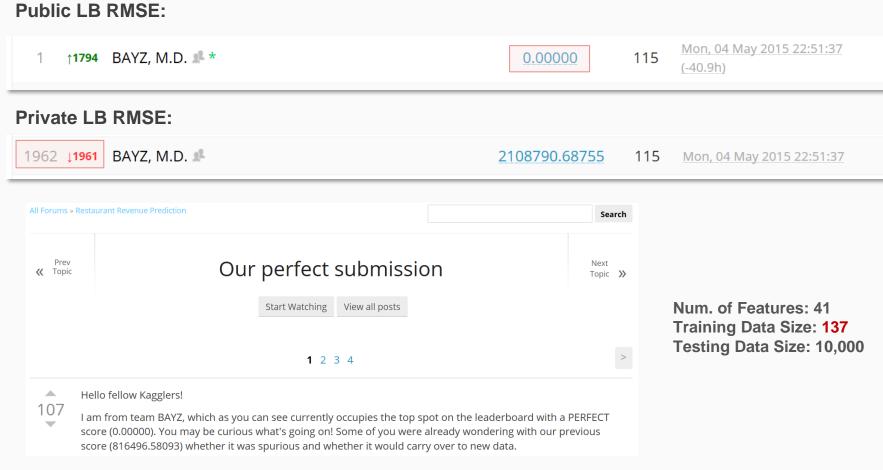


## Big Shake Up on Private LB!



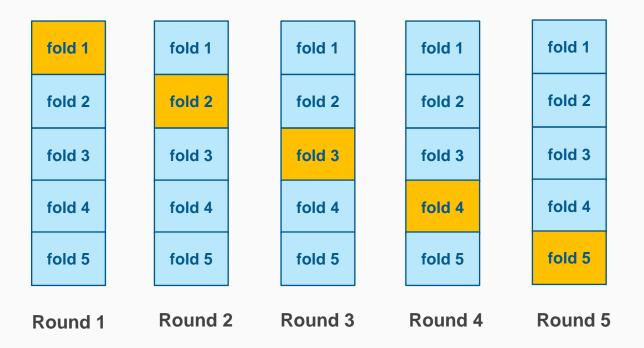
Reference: https://www.kaggle.com/c/restaurant-revenue-prediction/leaderboard/private

## Who is the King of Overfitting?

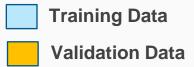


They even wrote a post to show off their perfect overfitting!

## K-fold Cross Validation (K = 5)



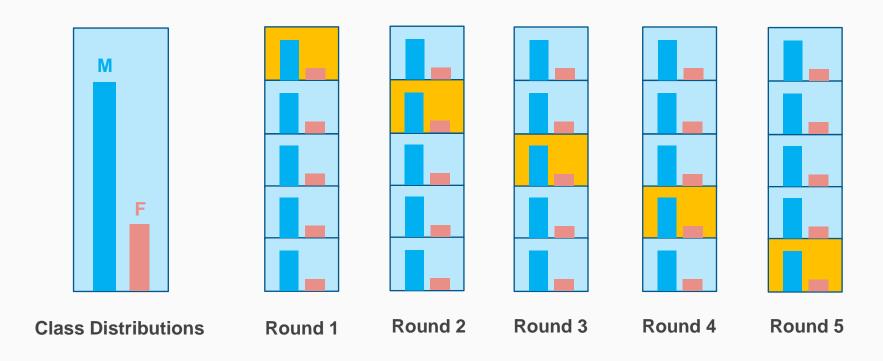
score(CV) = the average of evaluation scores from each fold You can also repeat the process many times!



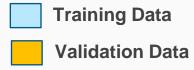
#### K-fold Cross Validation Tips

- It is normal to experience big shake up on private LB if not using local CV correctly
- 5 or 10 folds are not always the best choices (you need to consider the cost of computation time for training models)
- Which K to choose?
  - Depends on your data
  - Mimic the ratio of training and testing in validation process
  - Find a K with lowest gap between local CV and public LB scores
- Standard deviation of K-fold CV score matters more than mean!
- Stratified K-fold CV is important for imbalanced dataset, especially for classification problems

#### Stratified K-fold Cross Validation (K = 5)



Keep the distribution of classes in each fold



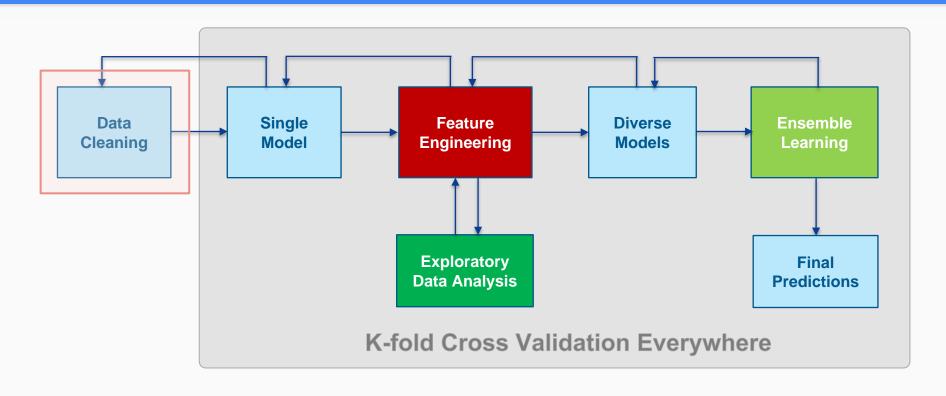
#### Should I Trust Public LB?

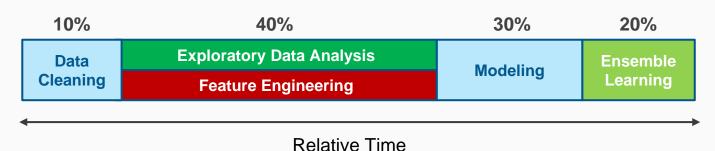
- Yes if you can find a K-fold CV that follows the same trend with public LB
  - High positive correlation between local CV and public LB
  - The score increases and decreases in both local CV and public LB
- Trust more in your local CV!

# Data Cleaning

Making data more analyzable

#### Recommended Data Science Process (IMHO)





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#### Data Cleaning Techniques

- Data cleaning is the removal of duplicates, useless data, or fixing of missing data
- Reduce dimensional complexity of dataset
  - Make training faster without hurting the performance
- Apply imputation methods to help (hopefully) utilize incomplete rows
  - Incomplete rows may contain relevant features (don't just drop them!)
  - In the risk of distorting original data, so be cautious!

- Remove duplicate features
  - Columns having the same value distribution or variance
  - Only need to keep one of them
- Remove constant features
  - Columns with only one unique value
  - R: sapply(data, function(x) length(unique(x)))
- Remove features with near-zero variance
  - R: nearZeroVar(data, saveMetrics=T) in caret package
- Be sure to know what you are doing before removing any features

- Some machine learning tools cannot accept NAs in the input
- Encode missing values to avoid NAs
  - Binary features
    - -1 for negatives, 0 for missing values and 1 for positives
  - Categorical features
    - Encode as an unique category
    - "Unknown", "Missing", ....
  - Numeric features
    - Encode as a big positive or negative number
    - 999, -99999, ....

- Basic ways to impute missing values
  - mean, median or most frequent value of feature
  - R: impute(x, fun = mean) in Hmisc package
  - Python: Imputer(strategy='mean', axis=0) in scikit-learn package

- Advanced: multiple imputation
  - Impute incomplete columns based on other columns in the data
  - R: mice package (Multivariate Imputation by Chained Equations)
- Imputation would not always give you positive improvements, thus you have to validate it cautiously

# Mostly Used Models

What models to use?

## Mostly Used ML Models

Model Type	Name	R	Python
Regression	Linear Regression	glm, glmnet	sklearn.linear_model.LinearRegression
	Ridge Regression	• glmnet	sklearn.linear_model.Ridge
	Lasso Regression	• glmnet	sklearn.linear_model.Lasso
Instance-based	K-nearest Neighbor (KNN)	• knn	sklearn.neighbors.KNeighborsClassifier
	Support Vector Machines (SVM)	svm {e1071}     LiblinearR	<ul> <li>sklearn.svm.SVC, sklearn.svm.SVR</li> <li>sklearn.svm.LinearSVC, sklearn.svm.LinearSVR</li> </ul>
Hyperplane-based	Naive Bayes	naiveBayes {e1071}	<ul><li>sklearn.naive_bayes.GaussianNB</li><li>sklearn.naive_bayes.MultinomialNB</li><li>sklearn.naive_bayes.BernoulliNB</li></ul>
	Logistic Regression	glm, glmnet     LiblinearR	sklearn.linear_model.LogisticRegression
Ensemble Trees	Random Forests	randomForest	<ul><li>sklearn.ensemble.RandomForestClassifier</li><li>sklearn.ensemble.RandomForestRegressor</li></ul>
	Extremely Randomized Trees	• extraTrees	<ul><li>sklearn.ensemble.ExtraTreesClassifier</li><li>sklearn.ensemble.ExtraTreesRegressor</li></ul>
	Gradient Boosting Machines (GBM)	<ul><li>gbm</li><li>xgboost</li></ul>	<ul> <li>sklearn.ensemble.GradientBoostingClassifier</li> <li>sklearn.ensemble.GradientBoostingRegressor</li> <li>xgboost</li> </ul>
Neural Network	Multi-layer Neural Network	<ul><li>nnet</li><li>neuralnet</li></ul>	PyBrain     Theano
Recommendation	Matrix Factorization	• NMF	• nimfa
	Factorization machines		• pyFM
Clustering	<i>K</i> -means	kmeans	sklearn.cluster.KMeans
	t-SNE	Rtsne	sklearn.manifold.TSNE

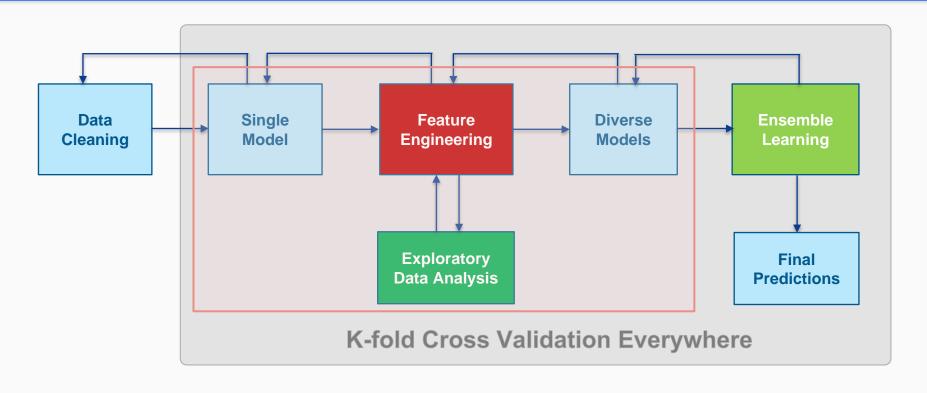
## Mostly Used ML Models (cont.)

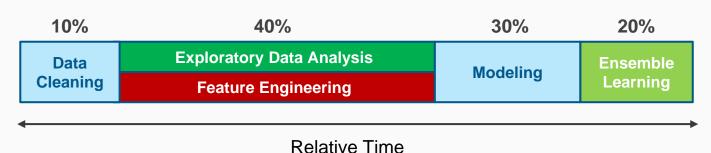
Model Type	Name	Mahout	Spark
Regression	Linear Regression		LinearRegressionWithSGD
	Ridge Regression		RidgeRegressionWithSGD
	Lasso Regression		LassoWithSGD
Instance-based	K-nearest Neighbor (KNN)		
	Support Vector Machines (SVM)		SVMWithSGD (only linearSVM)
Hyperplane-based	Naive Bayes	<ul><li>trainnb</li><li>spark-trainnb</li></ul>	NaiveBayes
	Logistic Regression	<ul><li>runlogistic</li><li>trainlogistic</li></ul>	<ul><li>LogisticRegressionWithLBFGS</li><li>LogisticRegressionWithSGD</li></ul>
Ensemble Trees	Random Forests	org.apache.mahout.classifier.df. mapreduce.BuildForest	RandomForest
	Extremely Randomized Trees		
	Gradient Boosting Machines (GBM)		GradientBoostedTrees
Neural Network	Multi-layer Neural Network		
Recommendation	Matrix Factorization	parallelALS	• ALS
	Factorization machines		
Clustering	<i>K</i> -means	• kmeans	KMeans
	t-SNE		

# Feature Engineering

The key to success

#### Recommended Data Science Process (IMHO)





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#### Feature Engineering

- Extract more new gold features, remove irrelevant or noisy features
  - Simpler models with better results
- The most important factor for the success of machine learning
- Key Elements
  - Data Transformation
  - Feature Encoding
  - Feature Extraction
  - Feature Selection

#### Data Transformation

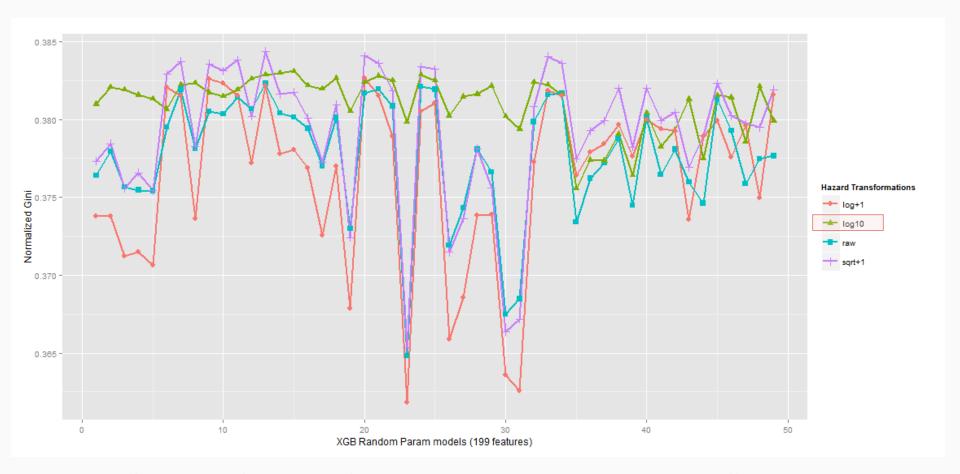
- Feature Scaling
  - Rescaling
    - Turn numeric features into the same scale (e.g., [-1,+1], [0,1], ...)
    - Python scikit-learn: MinMaxScaler
  - Standardization
    - Removing the mean ( $\mu = 0$ ) and scaling to unit variance ( $\sigma = 1$ )
    - Python scikit-learn: StandardScaler
    - R: scale
  - To avoid features in greater numeric ranges dominating those in smaller numeric ranges
  - Critical for regularized linear models, KNN, SVM, K-Means, etc.
  - Can make a big difference to the performance of some models
  - Also speed up the training of gradient decent
  - But not necessary to do it for tree-based models

#### Data Transformation (cont.)

- Predictor/Response Variable Transformation
  - Use it when variable shows a skewed distribution
  - make the residuals more close to "normal distribution" (bell curve)
  - Can improve model fit
  - log(x), log(x+1), sqrt(x), sqrt(x+1), etc.

#### Variable Transformation

In Liberty Mutual Group: Property Inspection Prediction



Different transformation of target response variable may lead to different results

#### Feature Encoding

- Turn categorical features into numeric features to provide more fine-grained information
  - Help explicitly capture non-linear relationships and interactions between the values of features
  - Some machine learning tools only accept numbers as their input
    - xgboost, gbm, glmnet, libsvm, liblinear, etc.

## Feature Encoding (cont.)

- Labeled Encoding
  - Interpret the categories as ordered integers (mostly wrong)
  - Python scikit-learn: LabelEncoder
- One Hot Encoding
  - Transform categories into individual binary (0 or 1) features
  - Python scikit-learn: DictVectorizer, OneHotEncoder
  - R: dummyVars in caret package

#### Feature Extraction: HTML Data

- HTML files are often used as the data source for classification problems
  - For instance, to identify whether a given html is an AD or not
- Possible features inside
  - html attributes (id, class, href, src, ....)
  - tag names
  - inner content
  - javascript function calls, variables, ....
  - script comment text
- Parsing Tools
  - Jsoup (Java), BeautyfulSoup (Python), etc.

#### Feature Extraction: Textual Data

- Bag-of-Words: extract tokens from text and use their occurrences (or TF/IDF weights) as features
- Require some NLP techniques to aggregate token counts more precisely
  - Split token into sub-tokens by delimiters or case changes
  - N-grams at word (often 2-5 grams) or character level
  - Stemming for English words
  - Remove stop words (not always necessary)
  - Convert all words to lower case
  - •
- Bag-of-Words Tools
  - R: tm package
  - Python: CountVectorizer, TfidfTransformer in scikit-learn package
  - Java: Lucene

#### Feature Extraction: Textual Data (cont.)

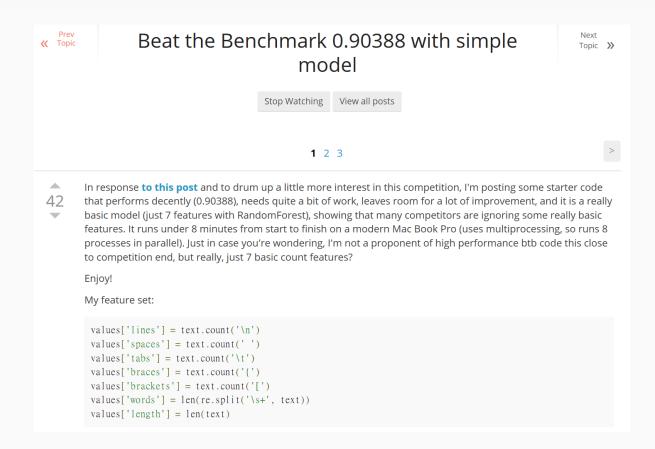
- Deep Learning for textual data
  - Turn each token into a vector of predefined size
  - Help compute "semantic distance" between tokens/words
    - For example, the semantic distance between user query and product titles in search results (how relevant?)
  - Greatly reduce the number of text features used for training
    - Use average vector of all words in given text
    - Vector size: 100~300 is often enough
  - Tools
    - Deeplearning4j (support Spark with GPUs)
      - Word2vec, Doc2vec
      - GloVe
    - Theano (support GPUs)

#### **Feature Extraction**

- There usually have some meaningful features inside existing features, you need to extract them manually
- Again you can use counts as features
- Some examples
  - Location
    - Address, city, state and zip code .... (categorical or numeric)
  - Time
    - Year, month, day, hour, minute, time ranges, .... (numeric)
    - Weekdays or weekend (binary)
    - Morning, noon, afternoon, evening, ... (categorical)
  - Numbers
    - Turn age numbers into ranges (ordinal or categorical)

## Feature Extraction: Simple But Powerful

 Counts of symbols and spaces inside text can also be powerful features!



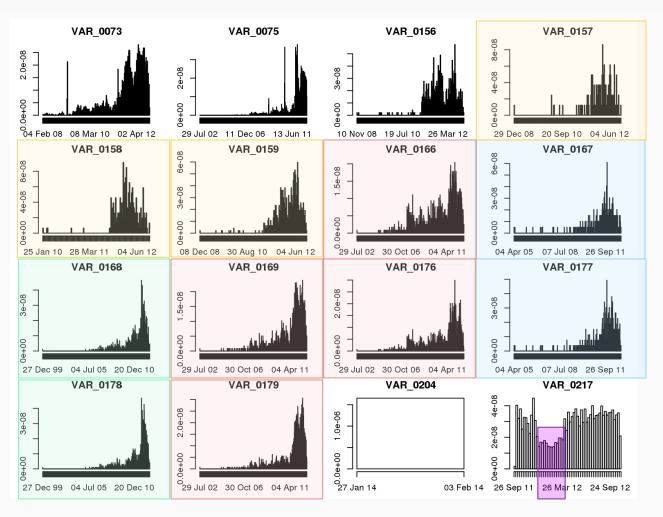
Using only 7 simple count features gives you over 0.90 AUC!

#### Feature Extraction: Hidden Features

- Sometimes there has some information leakage in the dataset provided by Kaggle competition
  - Timestamp information of data files
  - Some incautiously left meta-data inside HTML or text
- May lead to unfair results, so normally I skip this kind of competitions!

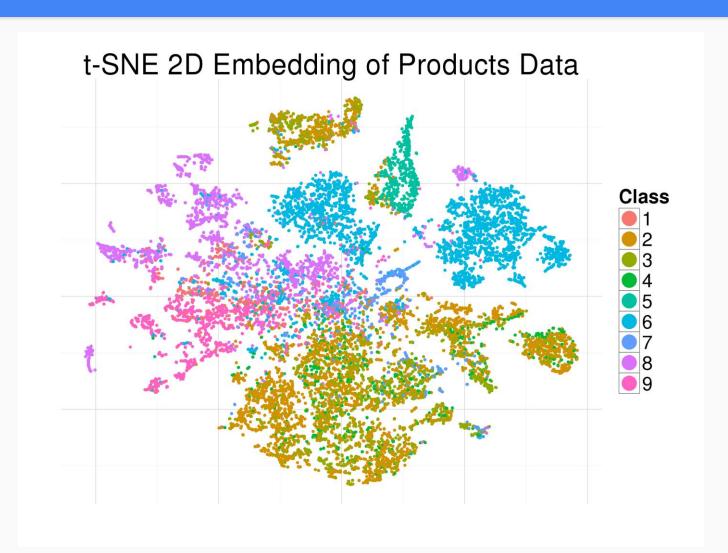
## Exploratory Data Analysis is Your Friend

Finding patterns and correlations from time series data



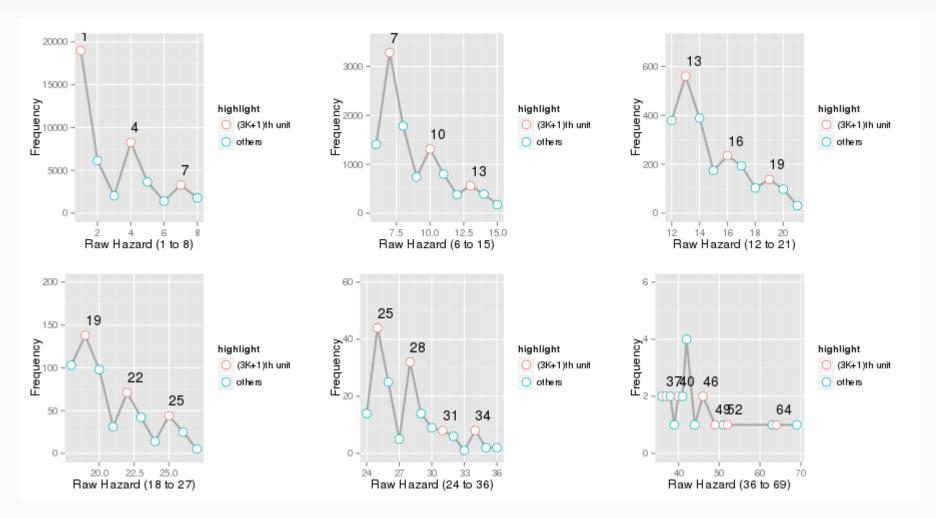
### Exploratory Data Analysis is Your Friend

Using 2D visualization to observe the distribution of data in problem space



## Exploratory Data Analysis is Your Friend

Finding hidden groups inside the data



Reference: https://www.kaggle.com/markpeng/liberty-mutual-group-property-inspection-prediction/hazard-groups-in-training-set/files

#### **Feature Selection**

- Reduce the number of features by removing redundant, irrelevant or noisy features
- Feature Explosion after Feature Extraction!
  - More than 100,000 unique token features from textual data is common
  - Hard to put all of them in memory!
  - PCA or truncated SVD can help to select top-N informative features
    - With the risk of ignoring non-linear relationships between features and dropping important features
    - Use them only if there is no other choice

## Feature Selection Methods

Type	Name	R	Python
Feature Importance Ranking	Gini Impurity	<ul><li>randomForest</li><li>varSelRF</li></ul>	<ul> <li>sklearn.ensemble.RandomForestClassifier</li> <li>sklearn.ensemble.RandomForestRegressor</li> <li>sklearn.ensemble.GradientBoostingClassifier</li> <li>sklearn.ensemble.GradientBoostingRegressor</li> </ul>
	Chi-square	Fselector	sklearn.feature_selection.chi2
	Correlation	Hmisc     Fselector	<ul><li>scipy.stats.pearsonr</li><li>scipy.stats.spearmanr</li></ul>
	Information Gain	<ul><li>randomForest</li><li>varSelRF</li><li>Fselector</li></ul>	<ul> <li>sklearn.ensemble.RandomForestClassifier</li> <li>sklearn.ensemble.RandomForestRegressor</li> <li>sklearn.ensemble.GradientBoostingClassifier</li> <li>sklearn.ensemble.GradientBoostingRegressor</li> <li>xgboost</li> </ul>
	L1-based Non-zero Coefficients	• glmnet	<ul><li>sklearn.linear_model.Lasso</li><li>sklearn.linear_model.LogisticRegression</li><li>sklearn.svm.LinearSVC</li></ul>
Feature Subset Selection	Recursive Feature Elimination (RFE)	rfe {caret}	sklearn.feature_selection.RFE
	Boruta Feature Selection	Boruta	
	Greedy Search (forward/backward)	Fselector	
	Hill Climbing Search	Fselector	
	Genetic Algorithms	gafs {caret}	

### **Feature Selection Methods**

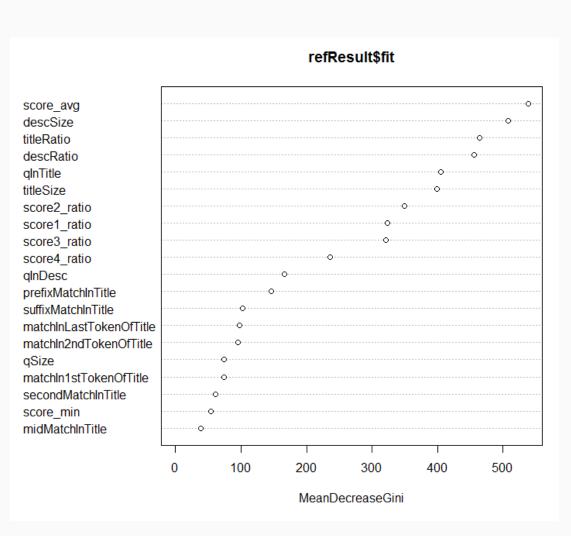
Туре	Name	Spark
Feature Importance Ranking	Gini Impurity	RandomForest (see <u>SPARK-5133</u> )
	Chi-square	ChiSqSelector
	Correlation	
	Information Gain	spark-mrmr-feature-selection
	L1-based Non-zero Coefficients	
	Recursive Feature Elimination (RFE)	
Feature Subset	Boruta Feature Selection	
Selection	Greedy Search (forward/backward)	
	Hill Climbing Search	
	Genetic Algorithms	

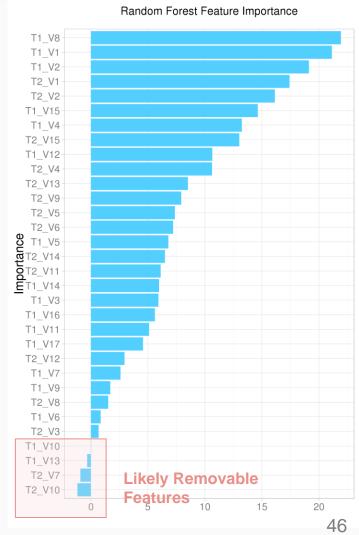
## Feature Importance (xgboost)



Reference: https://www.kaggle.com/tqchen/otto-group-product-classification-challenge/understanding-xgboost-model-on-otto-data/notebook

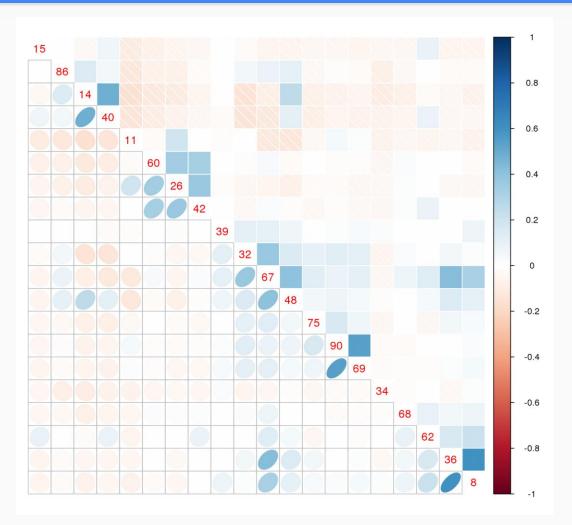
## Feature Importance (randomForest in R)





#### **Feature Correlations**

Correlations between top-20 features



Hypothesis: "Good feature subsets contain features highly correlated with the classification, yet uncorrelated to each other." - Wikipedia

Reference: https://www.kaggle.com/benhamner/otto-group-product-classification-challenge/important-feature-correlations

## Recursive Feature Elimination (RFE)

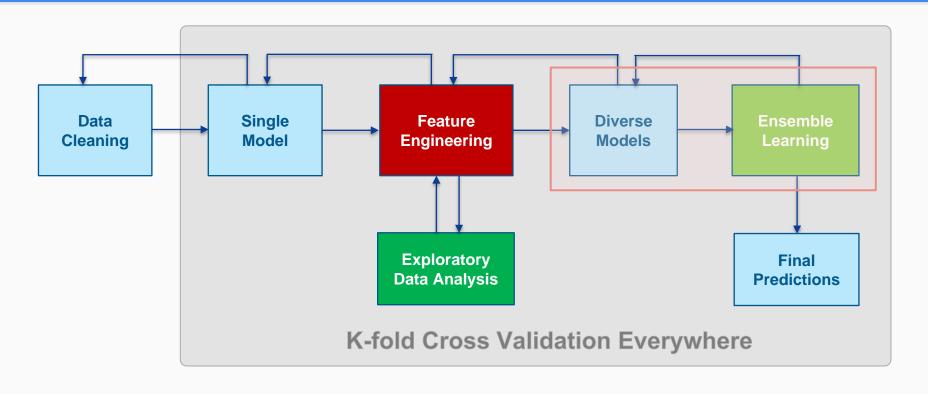
```
Recursive feature selection
   Outer resampling method: Cross-Validated (3 fold, repeated 3 times)
   Resampling performance over subset size:
 8
    Variables wKappa wKappaSD Selected
 9
            50 0.6715 0.008026
10
          100 0.6732 0.008263
11
          150 0.6773 0.007482
12
           200 0.6753 0.008301
13
           250 0.6762 0.007253
14
           300 0.6749 0.006091
15
           350 0.6741 0.006806
16
           400 0.6743 0.006093
17
           450 0.6756 0.004383
18
           500 0.6716 0.006937
19
           550 0.6743 0.008261
20
           600 0.6746 0.008223
21
           625 0.6731 0.007996
22
23 The top 5 variables (out of 150):
24
      C 377, C 417, C 381, C 379, C 457
```

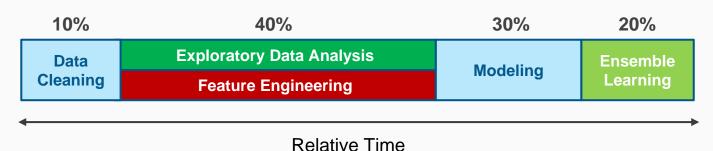
Find a subset of features with best performance

# **Ensemble Learning**

Beat single strong models

## Recommended Data Science Process (IMHO)

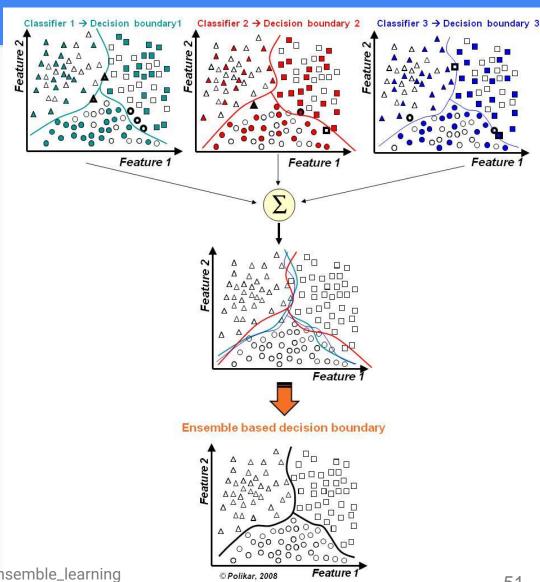




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## **Ensemble Learning - Illustration**

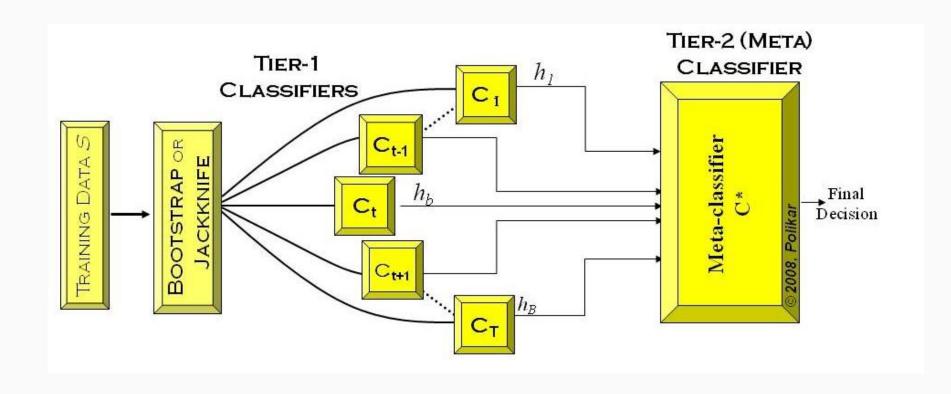
- Assume that diverse models see different aspects of the problem space and are wrong in different ways
- Simplest way: the average (possibly weighted) of model predictions
- Less variance
- Less generalization error
- Less chance of overfitting
- Better chance to win!



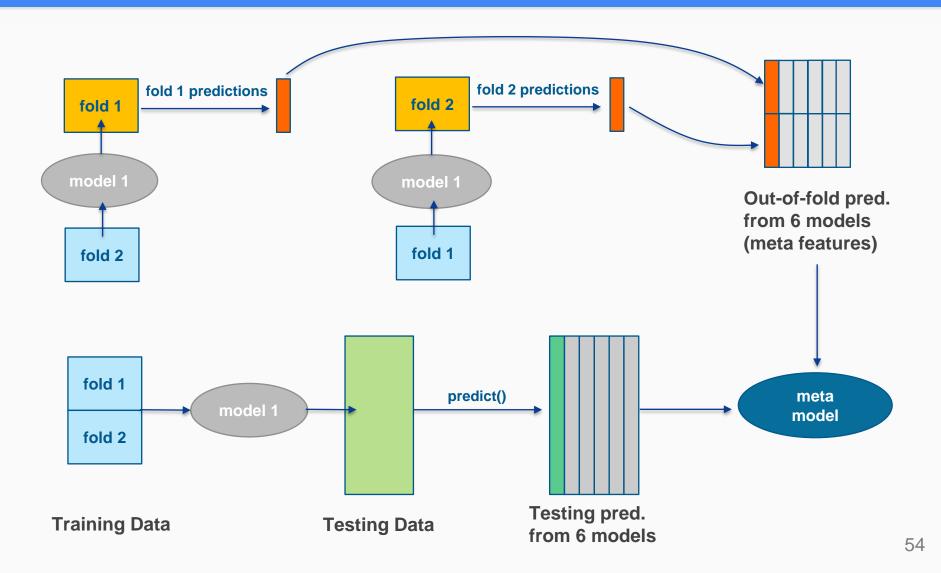
## Ensemble Learning - Stacked Generalization

- Using the predictions of current level models as features for training next level models
  - What we called "out-of-fold predictions" or "meta-features"
- Usually we only build 2 levels of models, 4 levels at most
- Can combine meta-features with original feature sets for training
- Potential risk of overfitting if cross validation process is not correct
- Also called "Stacking"
- Aims to reduce Generalization Error

## Ensemble Learning - Stacked Generalization



## Out-of-fold Prediction (K = 2)



#### **Out-of-fold Prediction - Generation Process**

- For example, 2-fold CV with 2 levels stacking
  - Split the train set into 2 parts: train\_fold1 and train\_fold2
  - Fit a first-level model on train\_fold1 and create predictions for train\_fold2
  - Fit the same model on train\_fold2 and create predictions for train\_fold1
  - Finally, fit the model again but on the entire training data, and create predictions for testing data
  - Using the predictions from the first-level model(s) as metafeatures, train a second-level model

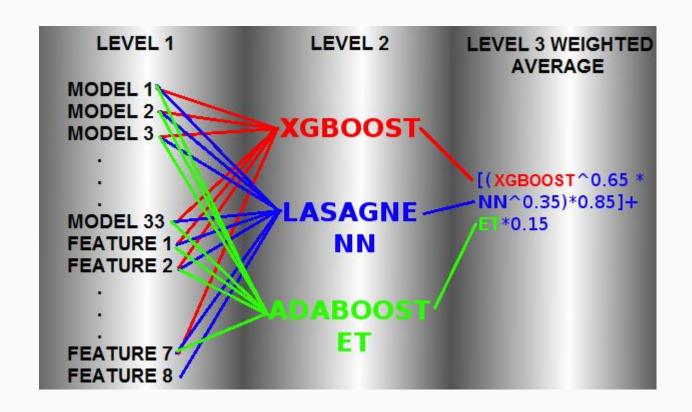
## Out-of-fold Prediction (cont.)

"I learned that you never, ever, EVER go anywhere without your out-of-fold predictions. If I go to Hawaii or to the bathroom I am bringing them with. Never know when I need to train a 2nd or 3rd level meta-classifier"

- T. Sharf

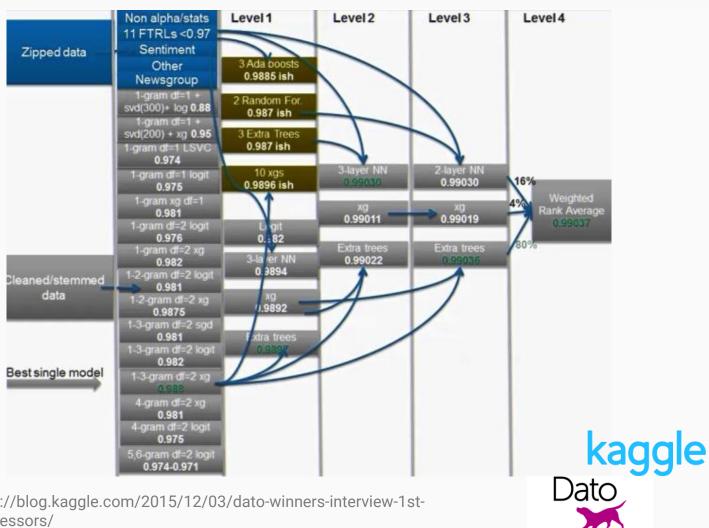
- Basic requirement for stacked generalization
- Can also combine with original features for modeling
- Keep it whenever building any models!

# Stacked Generalization Used by Gilberto Titericz Junior (new #1) in Otto Product Classification Challenge

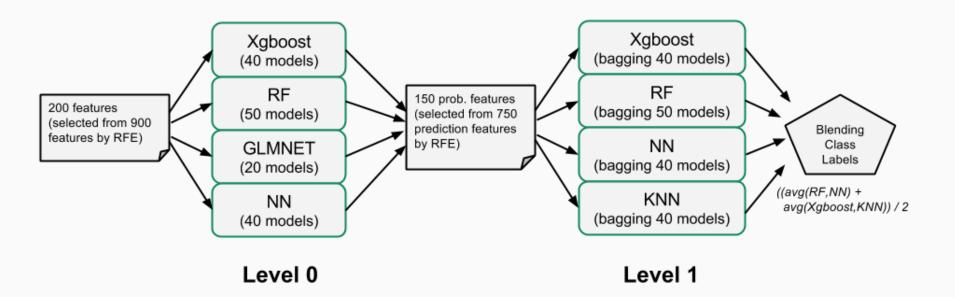




#### Stacked Generalization Used by the Winning Team in Truly Native? Competition (4 levels)



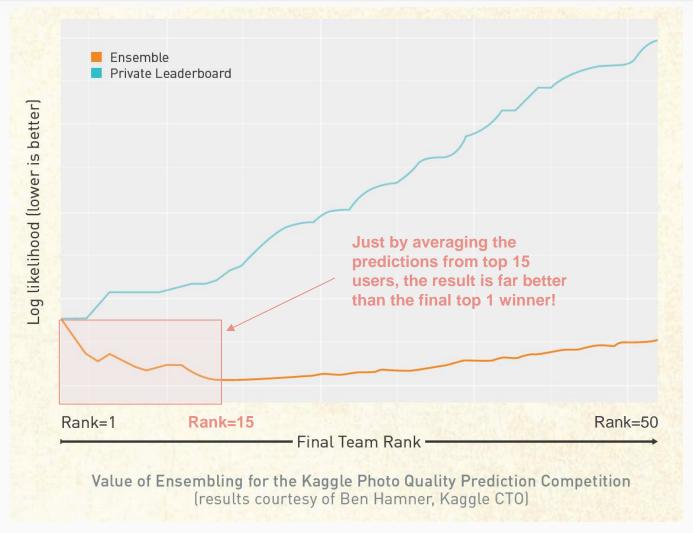
# Stacked Generalization I Used in Search Results Relevance Competition



More technical details can be found in this post: <a href="https://www.linkedin.com/pulse/ideas-sharing-kaggle-crowdflower-search-results-relevance-mark-peng">https://www.linkedin.com/pulse/ideas-sharing-kaggle-crowdflower-search-results-relevance-mark-peng</a>



## The Power of Ensemble Learning



## **Ensemble Learning - Tips**

- Always start from simple blending first
- Even simple bagging of multiple models of the same type can help reduce variance
- Generally work well with less-correlated good models
  - Models with similar performance but their correlation lies in between 0.85~0.95
  - Gradient Boosting Machines usually blend well with Random Forests

Must Read: Kaggle Ensembling Guide

# Team Up

Working with clever data geeks worldwide

## The Advantages of Team Up

- Fewer work loads for each one if divides up the work well
  - A focuses on feature engineering
  - B focuses on ensemble learning
  - C focuses on blending submissions
  - •
- Each member can contribute some single models for blending and stacking

## Ways to Team Up

#### Team up with some known friends

- Pros
  - Easy to discuss the ideas
  - Easy to divide up the work
  - Easy to share codes
- Cons
  - Harder to think outside the box because each one's ideas and thoughts might be tied together

## Ways to Team Up (cont.)

- Team up with other competitors worldwide (recommended)
  - Pros
    - You will learn a lot from the others from different counties and diverse background
    - Feature sets and models are less-correlated, thus more likely to produce better predictions after blending or stacking
    - Easier to finish with the Top 10
  - Cons
    - Harder to discuss the ideas (through emails or instant messages)
    - Harder to divide up the work
    - More sleepless!
  - Cloud storage can help share feature sets and codes

## When to Start Team Merger?

- Usually, each competition only allows 3 or 5 submissions per day per competitor
- After team merger, you have to share the quota with others in the team
- Combined team must have a total submission count less than or equal to the maximum allowed as of the merge date
- A better strategy (IMHO)
  - Start team merger 1-2 weeks before merger deadline
  - Give everyone enough daily submission to twist his/her mind and try out more ideas until exhausted

Good time to merge!

Merger and 1st Submission Deadline

#### How to Produce Better Predictions

- Feature Set Sharing
  - Rebuild everyone's models using others' feature set
  - More good single models for blending
- Blending Submissions
  - The easiest way to boost your team's ranking in LB
  - Weighted average often gives better LB score
  - Tune model weightings by handcrafting
- Multi-level Stacking based on Out-of-fold Predictions
  - Have to ask everyone build models using the same K folds and provide good out-of-fold predictions
  - Require more time and resources to train models in parallel
  - Produce the most powerful predictions!

## Recommended Resources

Materials to help you learn by doing

#### Books

- James G., Witten D., Hastie T., Tibshirani R. (2014). "An Introduction to Statistical Learning: with Applications in R," http://www-bcf.usc.edu/~gareth/ISL/
  - Many R examples to learn, good for the beginners
- Hastie T., Tibshirani R., Friedman J. (2009). "The Elements of Statistical Learning: Data Mining, Inference, and Prediction," http://statweb.stanford.edu/~tibs/ElemStatLearn/
  - Fundamental theories to statistics and machine learning
- Leskovec J., Rajaraman A., Ullman J. (2014). "Mining of Massive Datasets," http://www.mmds.org
  - How to scale data mining and machine learning to large dataset
- Booz Allen Hamilton. (2015). "Field Guide to Data Science," <a href="http://www.boozallen.com/insights/2015/12/data-science-field-guide-second-edition">http://www.boozallen.com/insights/2015/12/data-science-field-guide-second-edition</a>
  - A good overview about Data Science (Describe -> Discover -> Predict -> Advise)

## Massive Online Open Courses (MOOCs)

- Machine Learning, Stanford Professor Andrew Ng, Coursera Inc.
- Mining Massive Datasets, Stanford University, Coursera Inc.
- Statistical Learning, Stanford University, Stanford Online
- The Analytics Edge, MIT, edX Inc.
  - Very practical, final exam is to compete with other students on Kaggle!
- Introduction to Big Data with Apache Spark, Berkeley, edX Inc.
- Scalable Machine Learning, Berkeley, edX Inc.





#### Other Resources

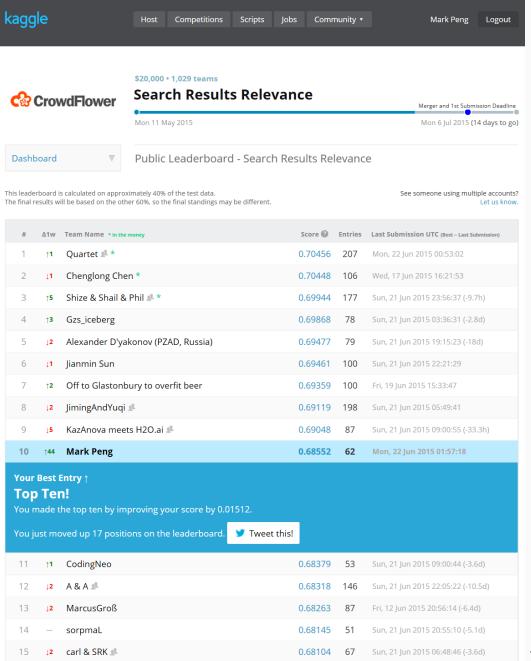
- Kaggle Competition Forums
  - https://www.kaggle.com/forums
  - Find similar competitions in the past
  - Pick out some code snippets and scripts shared by the others
  - Reading winners' codes is one of the best ways to learn
- "Winning Data Science Competitions" by Owen Zhang
- "A Few Useful Things to Know about Machine Learning" by Pedro Domingos
- "Advice for applying Machine Learning" by Andrew Ng

#### **Believe in Yourself**

You can make it to the 10 top along as well!

#### Then Team Up!

Prove yourself to team up with clever guys from all over the world



## **Concluding Words**

- "Think more, try less" by Owen Zhang
- Find a competition with the dataset you loved
- Build your own reusable toolkit and framework for CV and modeling
- Use fixed seeds to make sure your results is reproducible
- Learn from Top Winners
- Be disciplined, focus on one competition at a time
- Data science is an iterative process
- Always trust more in your local CV!

## Thanks!

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