Kaggle Competitions 101

The Airbnb of Data Scientists

AGENDA

- **Anatomy of a Kaggle Competition [10-15 mins]**
  - Competition Mechanics
  - Register, download data, and access kaggle notebooks
- **Let's Ensemble [60 mins]**
  - Algorithms, tools, and frameworks in perspective
- **Competition- House Prices Advanced Regression [30 mins]**

GOALS

- Get familiar with the mechanics of Data Science Competitions
- Get comfortable with the Kaggle Kernel environment
- Familiarise with algorithms behind most Kaggle winning solutions
- **At the end of this tutorial:**
  - Submitted at least 2 entries to a Kaggle competition
  - Applied Algorithms on Kaggle Data
    - Gradient Boosting Machines, Xgboost, Model Averaging and Model Stacking

TUTORIAL MATERIAL

go.ncsu.edu/kaggle
(slides+notebooks)

ANATOMY OF KAGGLE COMPETITIONS

COMPETITION CONCEPTS

- Data
- Model
- Submission (only predictions)
- Evaluation function— RMSE, Logloss, Mean Absolute Error, ROCAUC, etc
- Leaderboard (Public/Private)
- Kernels

PUBLIC/PRIVATE TESTS

BEHIND THE MEDALS (1/2)

BEHIND THE MEDALS (2/2)

LET'S ENSEMBLE

An ode to Leo Brieman

DATASET: PIMA INDIANS DIABETES

Attribute Characteristics: Integer	**Missing Values:** Yes	DataSet Characteristic: Univariate
No. of Instances: 768	**Evaluation Metric:** Accuracy	Area: Medical
No of Attributes: 8	**Associate Tasks:** Classification	Link: Pima Indians Diabetes Dataset

EXAMPLE- WINNING SOLUTIONS

STACKING EXAMPLE

REAL WORLD ML PIPELINE

MODERN MACHINE LEARNING LANDSCAPE

- Since 2016, Kaggle has been dominated by two approaches:
  - Gradient Boosting Machines
  - Deep Learning

(And Combined Models (eg. Voting, Averaging, and Stacking))

OUR ROADMAP

Bias related errors
Adaptive boosting
Gradient boosting
dmlc
XGBoost
Bagging
Random forest
Variance related errors

DECISION TREE

- Nodes are split by finding the best split.
- For classification, entropy or gini entropy are criteria for measuring impurity of a node.
- For regression, we use mean squared error.
- Pros and Cons

PREDICTIVE ANALYSIS

Supervised Learning: y= f(x), f is unknown.

GOALS OF SUPERVISED LEARNING

- Find a model $\hat{f}$ that best approximates f: $f \approx \hat{f}$
- $\hat{f}$ can be Linear Regression, KNN, Decision Tree, Neural Networks, etc..
- Discard noise as much as possible
- **End goal:** $\hat{f}$ should receive a low predictive error on unseen data

DIFFICULTIES IN APPROXIMATING F

- **Overfitting**

$\hat{f}(x)$ fits the training set noise

- **Underfitting**

$\hat{f}$ is not flexible enough to approximate

GENERALIZATION ERROR

- Generalisation error of $\hat{f}$: Does generalise well on unseen data?
- It can be decomposed as follows:
  - Generalisation Error of $\hat{f}$: $Bias^2$ + Variance + irreducible error

BIAS

- Error term that tells you, on average how much $\hat{f} \neq f$

VARIANCE

- Tells you how much $\hat{f}$ is inconsistent over different training sets.

BIAS-VARIANCE TRADEOFF

ESTIMATING THE GENERALISATION ERROR

- How do we estimate the generalisation error of a model?
- Cannot be done directly because:
  - f is unknown
  - usually you only have one dataset
  - noise is unpredictable
- Solution: train-test split, K-fold, CV fold

BAGGING (1/2)

- Introduced by Leo Breiman in 1996 as a method to reduce model variance.
- Also called Bootstrap Aggregation
- Fit many large trees to bootstrap-resampled version of the training data, to classify by majority voting.
- Bias of individual trees increases slightly
- But that is compensated by averaging slightly different versions of the same model, which has the effect of reducing variance, thereby improve accuracy.

BAGGING (2/2)

Tree
Bagging(Tree)
f(x)
LS ~ y = f(x) + noise
ŷ(x)
$\mathbb{E}_{LS}\hat{y}(x)$
error(x)
bias²(x)
variance(x)
noise(x)

RANDOM FORESTS

- Each tree is built from samples drawn with replacement from the training set.
- Nodes are split by finding the best split among a random subset of features.
- As a result of this randomness, bias of the result slightly increases (w.r.t. the bias of a single non-random tree) but due to averaging its variance also decreases.

ROADMAP REVISITED

BOOSTING

A form of weighted averaging of models where each model is built sequential via taking into account the past model performance.

Main Boosting types:

- Weight based (Adaboost)
- Residual based (GBM)

ADABOOST

Rownum	x0	x1	x2	x3	y	pred	abs.error	weight
0	0.94	0.27	0.80	0.34	1	0.80	0.20	1.20
1	0.84	0.79	0.89	0.05	1	0.75	0.25	1.25
2	0.83	0.11	0.23	0.42	1	0.65	0.35	1.35
3	0.74	0.26	0.03	0.41	0	0.40	0.40	1.40
4	0.08	0.29	0.76	0.37	0	0.55	0.55	1.55
5	0.71	0.76	0.43	0.95	1	0.34	0.66	1.66
6	0.08	0.72	0.97	0.04	0	0.02	0.02	1.02

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RESIDUAL BASED BOOSTING

Rownum	x0	x1	x2	x3	y	pred	error
0	0.94	0.27	0.80	0.34	1	0.80	0.20
1	0.84	0.79	0.89	0.05	1	0.75	0.25
2	0.83	0.11	0.23	0.42	1	0.65	0.35
3	0.74	0.26	0.03	0.41	0	0.40	-0.40
4	0.08	0.29	0.76	0.37	0	0.55	-0.55
5	0.71	0.76	0.43	0.95	1	0.34	0.66
6	0.08	0.72	0.97	0.04	0	0.02	-0.02

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EXAMPLE (CONT)

Rownum	x0	x1	x2	x3	y	new pred	old pred
0	0.94	0.27	0.80	0.34	0.2	0.15	0.80
1	0.84	0.79	0.89	0.05	0.25	0.20	0.75
2	0.83	0.11	0.23	0.42	0.35	0.40	0.65
3	0.74	0.26	0.03	0.41	-0.4	-0.30	0.40
4	0.08	0.29	0.76	0.37	-0.55	-0.20	0.55
5	0.71	0.76	0.43	0.95	0.66	0.24	0.34
6	0.08	0.72	0.97	0.04	-0.02	-0.01	0.02

To predict Rownum=1 we would say :

Final prediction = 0.75 + 0.20 = **0.95**

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RESIDUAL BASED BOOSTING PARAMETERS

- Learning rate (shrinkage)
- Number of estimators
- Row (sub) sampling
- Column (sub) sampling
- Input model- better be trees

RESIDUAL BASED IMPLEMENTATIONS

- Xgboost
- Lightgbm
- H2O's GBM
- CatBoost
- Sklearn's GBM

COMBINING MODELS

- Get additional performance gains by combining strong models made with different algorithms.

COMBINING MODELS

- Three typical ways to combine models are:
  - Averaging
    - Simple Averaging
    - Weighted Averaging
    - Conditional Averaging
  - Majority Voting
  - Stacking

AVERAGING EXAMPLE

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SIMPLE AVERAGING

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WEIGHTED AVERAGING

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CONDITIONAL AVERAGING

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VOTING CLASSIFIERS (1/2)

- Binary Classification task
- Meta-Model prediction: **hard voting** (also known as majority voting).

VOTING CLASSIFIERS (2/2)

- In **soft voting**, every individual classifier provides a probability value that a specific data point belongs to a particular target class. The predictions are weighted by the classifier's importance and summed up. Then the target label with the greatest sum of weighted probabilities wins the vote.

classifier	class 0	class 1
classifier #1	$0.3\ w_1$	$0.7\ w_1$
classifier #2	$0.5\ w_2$	$0.5\ w_2$
classifier #3	$0.4\ w_3$	$0.6\ w_3$

STACKING

Making predictions of a number of models on a hold-out set and then using a different (meta) model to train on these predictions.

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STACKING EXAMPLE

A

X0	x1	x2	xn	y
0.17	0.25	0.93	0.79	1
0.35	0.61	0.93	0.57	0
0.44	0.59	0.56	0.46	0
0.37	0.43	0.74	0.28	1
0.96	0.07	0.57	0.01	1

B

X0	x1	x2	xn	y
0.89	0.72	0.50	0.66	0
0.58	0.71	0.92	0.27	1
0.10	0.35	0.27	0.37	0
0.47	0.68	0.30	0.98	0
0.39	0.53	0.59	0.18	1

C

X0	x1	x2	xn	y
0.29	0.77	0.05	0.09	?
0.38	0.66	0.42	0.91	?
0.72	0.66	0.92	0.11	?
0.70	0.37	0.91	0.17	?
0.59	0.98	0.93	0.65	?

Train algorithm **0** on A and make predictions for B and C and save to **B1**, **C1**
Train algorithm **1** on A and make predictions for B and C and save to **B1**, **C1**
Train algorithm **2** on A and make predictions for B and C and save to **B1**, **C1**

B1

pred0	pred1	pred2	y
0.24	0.72	0.70	0
0.95	0.25	0.22	1
0.64	0.80	0.96	0
0.89	0.58	0.52	0
0.11	0.20	0.93	1

C1

pred0	pred1	pred2	y	Preds3
0.50	0.50	0.39	?	0.45
0.62	0.59	0.46	?	0.23
0.22	0.31	0.54	?	0.99
0.90	0.47	0.09	?	0.34
0.20	0.09	0.61	?	0.05

Train algorithm **3** on B1 and make predictions for C1

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METHODOLOGY

- Wolpert introduced stacking in 1992. It involves:

1. Splitting the train set into two disjoint sets.
2. Train several base learners on the first part (train set).
3. Make predictions with base learners on the second part (validation set).
4. Using the predictions from the previous step as inputs to train a higher level learner.

```
#split train data in 2 parts, training and  valdiation.
training,valid,ytraining,yvalid = train_test_split(train,y,test_size=0.5)
#specify models
model1=RandomForestRegressor()
model2=LinearRegression()
#fit models
model1.fit(training,ytraining)
model2.fit(training,ytraining)
#make predictions for validation
preds1=model1.predict(valid)
preds2=model2.predict(valid)
#make predictions for test data
test_preds1=model1.predict(test)
test_preds2=model2.predict(test)
#Form a new dataset for valid and test via stacking the predictions
stacked_predictions=np.column_stack((preds1,preds2))
stacked_test_predictions=np.column_stack((test_preds1,test_preds2))
#specify meta model
meta_model=LinearRegression()
#fit meta model on stacked predictions
meta_model.fit(stacked_predictions,yvalid)
#make predictions on the stacked predictions of the test data
final_predictions=meta_model.predict(stacked_test_predictions)
```

HOW TO TRAIN (1/4)

For large datasets:

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HOW TO TRAIN (2/4)

We use K-fold CV

Fold 1

x0	x1	x2	x3	y
0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

Predict

Train

pred
0.96
0.03
0.00
0.00
0.00
0.00
0.00
0.00

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HOW TO TRAIN (3/4)

Fold 1

x0	x1	x2	x3	y
0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

Predict

Train

pred
0.96
0.03
0.90
0.12
0.00
0.00
0.00
0.00

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HOW TO TRAIN (4/4)

x0	x1	x2	x3	y
0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1
0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

Predict

0.08	0.72	0.97	0.04	0
0.84	0.79	0.89	0.05	1

Train

0.94	0.27	0.80	0.34	1
0.02	0.22	0.17	0.84	0
0.83	0.11	0.23	0.42	1
0.74	0.26	0.03	0.41	0
0.08	0.29	0.76	0.37	0
0.71	0.76	0.43	0.95	1

test
0.43
0.03
0.90
0.12
0.03
0.77
0.18
0.91

pred	pred
0.96	0.00
0.03	0.00
0.90	0.00
0.12	0.00
0.03	0.00
0.77	0.00
0.18	0.00
0.91	0.00

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THINGS TO BE MINDFUL OF

- With time sensitive data—respect time
- Diversity as important as performance
- Diversity may come from
  - Different algorithms
  - Different input features
- Performance plateauing after N models

NAIVE EXAMPLE

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HOMESITE-WINNING SOLUTION

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ON TO COMPETITIONS

HOUSE PRICES: ADVANCED REGRESSION TECHNIQUES

DATASET: HOUSE PRICES COMPETITION

DataSet Characteristics: Multivariate	**Attribute Characteristics:** Integer	**Associate Tasks:** Regression
No. of Instances: 1460	**Missing Values:** Yes	**Area:** Real-Estate
No of Attributes: 79	**Evaluation Metric:** RMSLE	**Link:** House Prices: Advanced Regression Techniques

Questions

Thank You