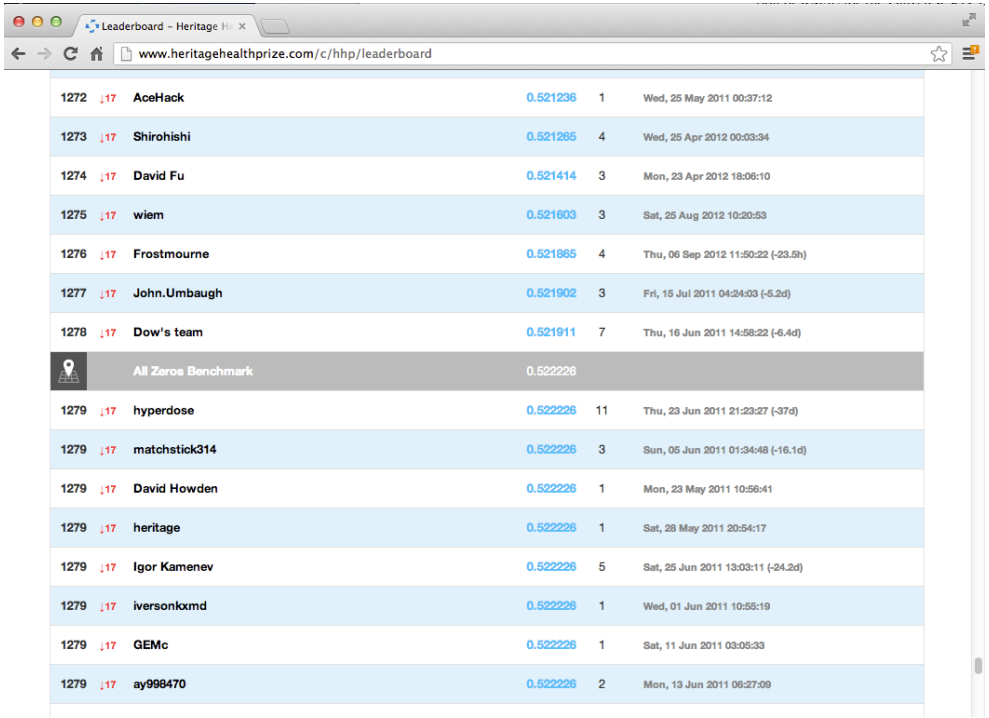
Prediction study design

Jeffrey Leek
Johns Hopkins Bloomberg School of Public Health

Prediction study design

1. Define your error rate
2. Split data into:
    - Training, Testing, Validation (optional)
3. On the training set pick features
    - Use cross-validation
4. On the training set pick prediction function
    - Use cross-validation
5. If no validation
    - Apply 1x to test set
6. If validation
    - Apply to test set and refine
    - Apply 1x to validation

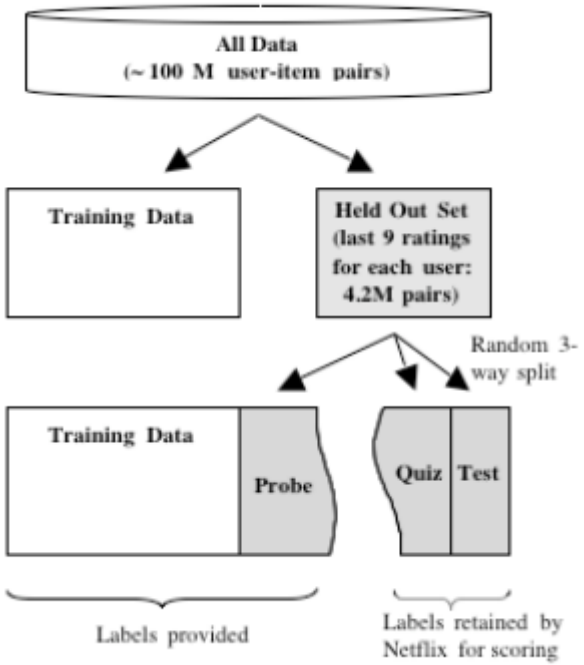
Know the benchmarks



1272	↓17	AceHack	0.521236	1	Wed, 25 May 2011 00:37:12
1273	↓17	Shirohishi	0.521265	4	Wed, 25 Apr 2012 00:03:34
1274	↓17	David Fu	0.521414	3	Mon, 23 Apr 2012 18:06:10
1275	↓17	wiem	0.521603	3	Sat, 25 Aug 2012 10:20:53
1276	↓17	Frostmourne	0.521865	4	Thu, 06 Sep 2012 11:50:22 (-23.5h)
1277	↓17	John.Umbaugh	0.521902	3	Fri, 15 Jul 2011 04:24:03 (-5.2d)
1278	↓17	Dow's team	0.521911	7	Thu, 16 Jun 2011 14:58:22 (-6.4d)
		All Zeros Benchmark	0.522226		
1279	↓17	hyperdose	0.522226	11	Thu, 23 Jun 2011 21:23:27 (-37d)
1279	↓17	matchstick314	0.522226	3	Sun, 05 Jun 2011 01:34:48 (-16.1d)
1279	↓17	David Howden	0.522226	1	Mon, 23 May 2011 10:56:41
1279	↓17	heritage	0.522226	1	Sat, 28 May 2011 20:54:17
1279	↓17	Igor Kamenev	0.522226	5	Sat, 25 Jun 2011 13:03:11 (-24.2d)
1279	↓17	iversonkxmd	0.522226	1	Wed, 01 Jun 2011 10:55:19
1279	↓17	GEMc	0.522226	1	Sat, 11 Jun 2011 03:05:33
1279	↓17	ay998470	0.522226	2	Mon, 13 Jun 2011 06:27:09

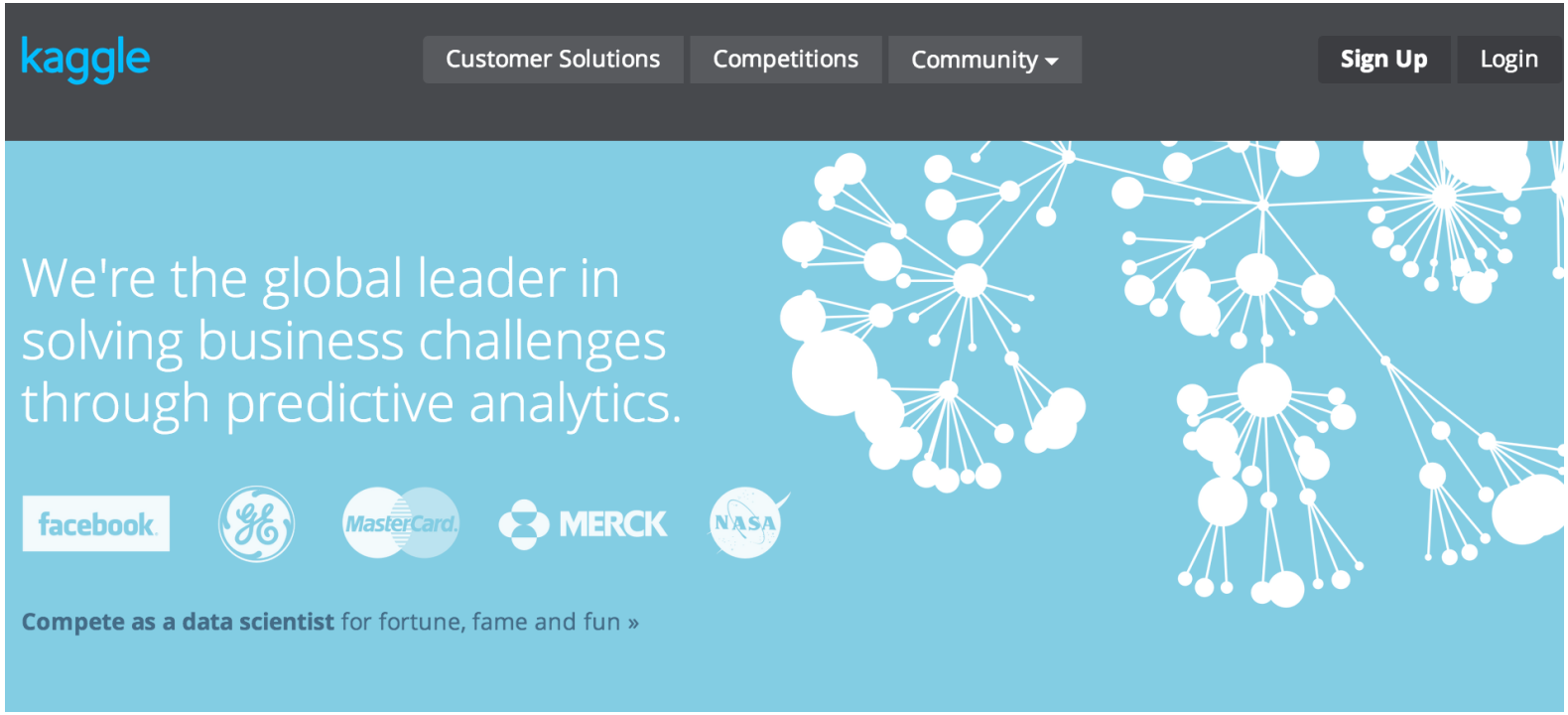
http://www.heritagehealthprize.com/c/hhp/leaderboard

Study design



http://www2.research.att.com/~volinsky/papers/ASAStatComp.pdf

Used by the professionals



http://www.kaggle.com/

Avoid small sample sizes

- Suppose you are predicting a binary outcome
  - Diseased/healthy
  - Click on ad/not click on ad
- One classifier is flipping a coin
- Probability of perfect classification is approximately:
  - $\left(\frac{1}{2}\right)^{sample\ size}$
  - $n = 1$ flipping coin 50% chance of 100% accuracy
  - $n = 2$ flipping coin 25% chance of 100% accuracy
  - $n = 10$ flipping coin 0.10% chance of 100% accuracy

Rules of thumb for prediction study design

- If you have a large sample size
  - 60% training
  - 20% test
  - 20% validation
- If you have a medium sample size
  - 60% training
  - 40% testing
- If you have a small sample size
  - Do cross validation
  - Report caveat of small sample size

Some principles to remember

- Set the test/validation set aside and *don't look at it*
- In general *randomly* sample training and test
- Your data sets must reflect structure of the problem
  - If predictions evolve with time split train/test in time chunks (calledbacktesting in finance)
- All subsets should reflect as much diversity as possible
  - Random assignment does this
  - You can also try to balance by features - but this is tricky