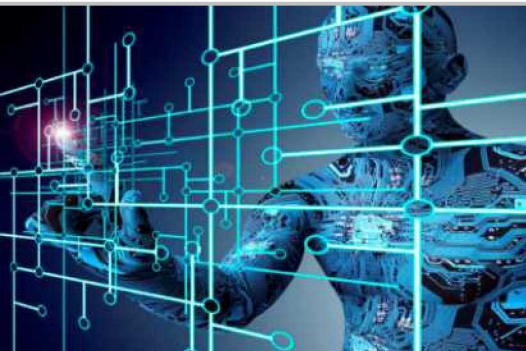


Designing for Interpretability and Adaptability  
by Using Weighted Averages

Sapan Agarwal  
Andrew De La Cruz  
Corey Hudson

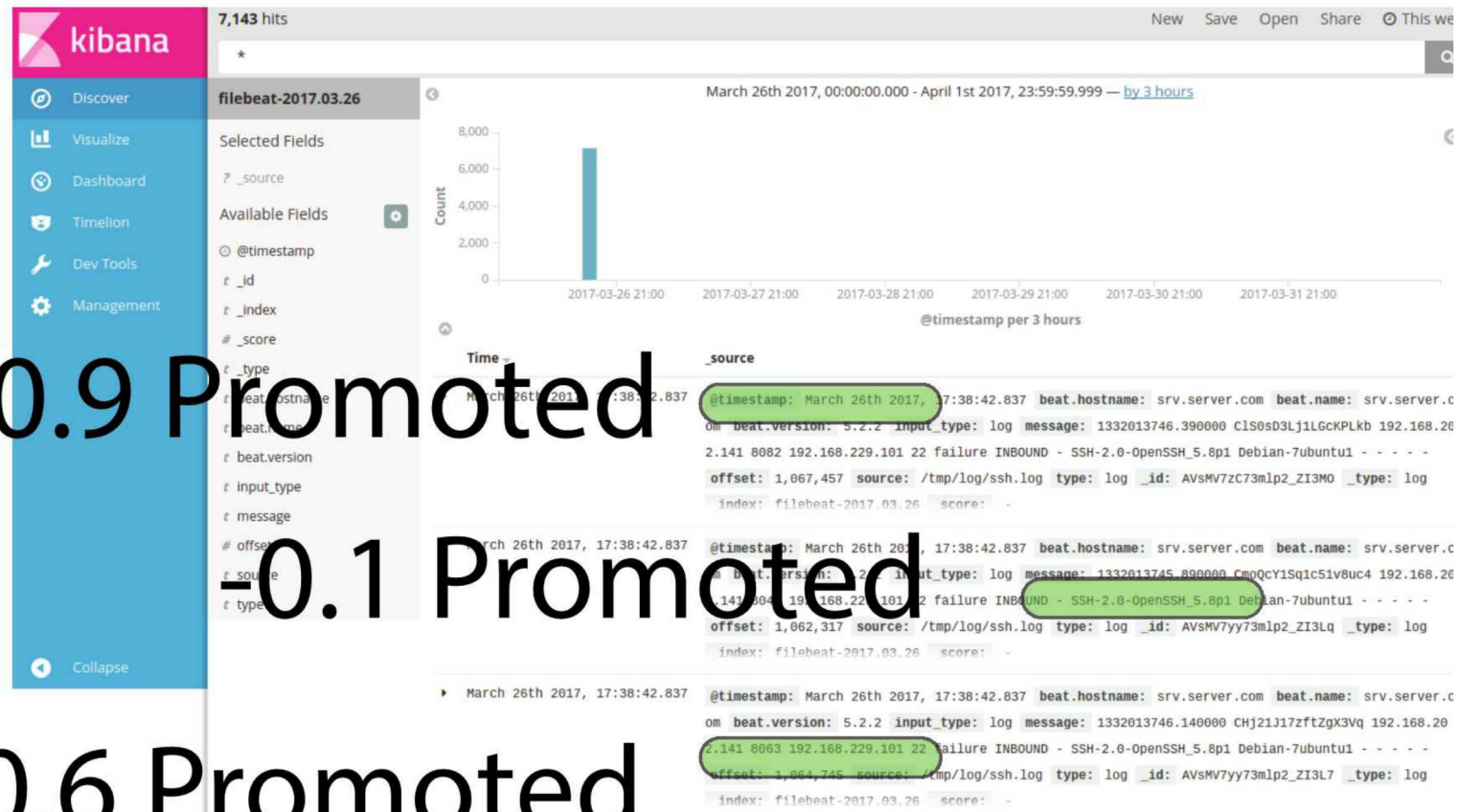


# Designing for Interpretability and Adaptability by Using Weighted Averages

**Sapan Agarwal, Andrew De La Cruz, Corey Hudson**

# Want to Highlight Key Features in an Alert

Use machine learning to classify or prioritize alerts and indicate what parts a human analyst should focus on



+0.9 Promoted

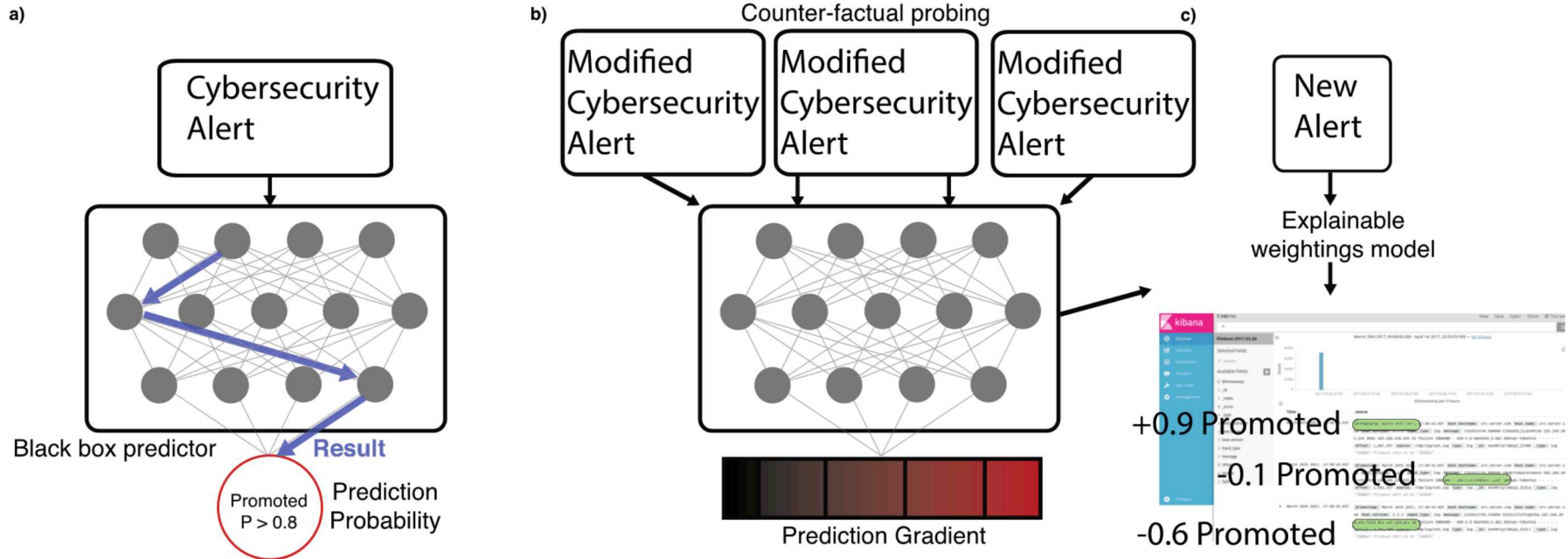
-0.1 Promoted

-0.6 Promoted

# Explainability background

- Explainability and accuracy are frequently at odds in classification and ranking problems
- Logistic regression is imminently explainable
- $\text{logit}(C) = \beta_0 + \sum_{i=1}^n \beta_i X_i$
- However...for even trivially simple examples, like MNIST (handwriting), LR scores about 93% accuracy vs record accuracies around 99.8%

# State of the art: Counterfactual probing



# Problem with Counterfactual Probing

1. Typically requires the model be mapped onto a linear model
2. Decision and explainability models are separate
3. Not scalable!!
4. Requires a robust sense of what randomization means for alerts



# Ideal classifier

1. Highly accurate
2. Explains each instance
3. Streaming, modifiable on the fly
4. Scalable

**Use our new classifier:**

**AWE-ML: Averaged Weights for Explainable  
Machine Learning**

# Want a Fast, Adaptable, Explainable Classifier

Find the probability of outcome  $Y = 1$   
given measured features  $x_1 = x_1', x_2 = x_2', x_3 = x_3'$

Estimate  $P(Y = 1 | x_1 = x_1', x_2 = x_2', x_3 = x_3')$

From training data, measure the following probabilities:

$$P(Y = 1) = 0.8$$

$$P(Y = 1 | x_1 = x_1') = 0.001$$

$$P(Y = 1 | x_2 = x_2') = 0.9$$

$$P(Y = 1 | x_3 = x_3') = 0.7$$

$$P(Y = 1 | x_1 = x_1', x_2 = x_2') = 0$$

How do we combine these to get the best overall probability estimate?

# No Good 1<sup>st</sup> Principles Method

- Bayesian methods degenerate to values of 0 and 1
- One route to determine the importance of features is by averaging the probabilities

$$P(Y = 1 | x_1 = x_1', x_2 = x_2', x_3 = x_3') \approx \frac{\sum_i P(Y=1 | x_i = x_i')}{\sum_i 1}$$

- Need to account for many effects:
  - Use combinations of features:  $P(Y = 1 | x_i = x_i', x_j = x_j')$
  - As a P approaches 0 or 1, it should be given more weight
  - Measured probabilities with less supporting data should be given less weight
  - Measured probabilities that give new information should possibly be given more weight
  - Account for class imbalance

$$P = \sum_i w_i \times P(Y = 1 | x_i = x_i') + \sum_{ij} w_{ij} \times P(Y = 1 | x_i = x_i', x_j = x_j') + \dots$$

Use a Hierarchical Weighted Average



# Using Categorical / Binned Data

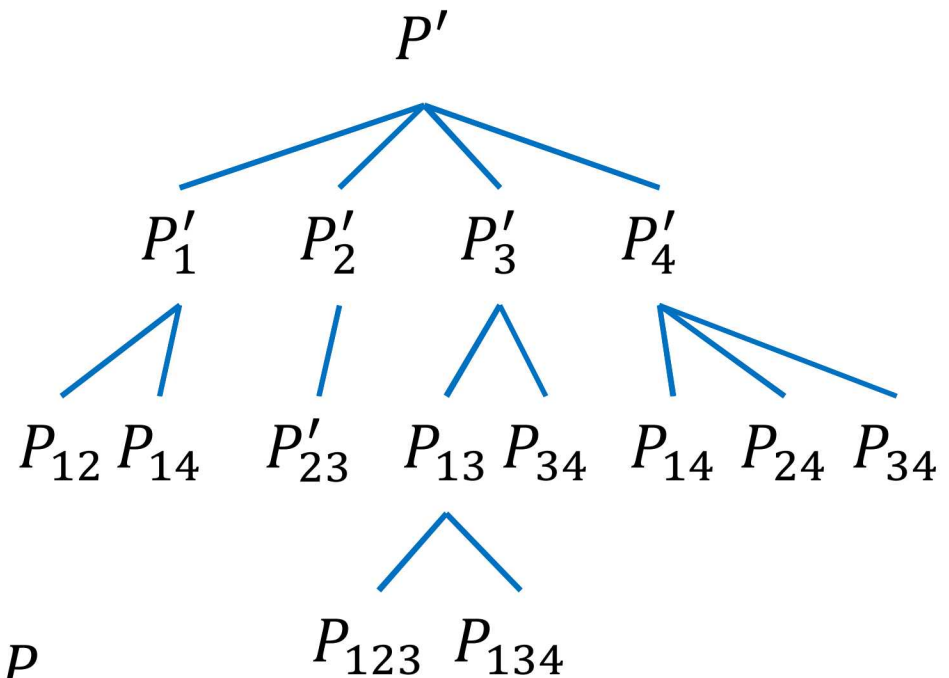
- AWE-ML requires data to be binned into categorical variables
- Binned data allows classifications to be directly tied to specific bins in the training data
- Random forests directly use continuous data averaged over different cuts of the data, preventing identification of the specific subset of the training data that is relevant to classification.
- Binning may result in a small loss in accuracy, but a gives a large improvement in explainability and adaptability.

# Hierarchically Average the Probability

$$P' = \frac{\sum_i P'_i}{\sum_i 1}$$

$$P'_i = \frac{\sum_{j \neq i} P'_{ij}}{\sum_{j \neq i} 1}$$

$$P'_{ij} = \frac{\sum_{k \neq j \neq i} P'_{ijk}}{\sum_{k \neq j \neq i} 1}$$



$P = P(Y = 1)$ ,  $P'$  = estimate of  $P$

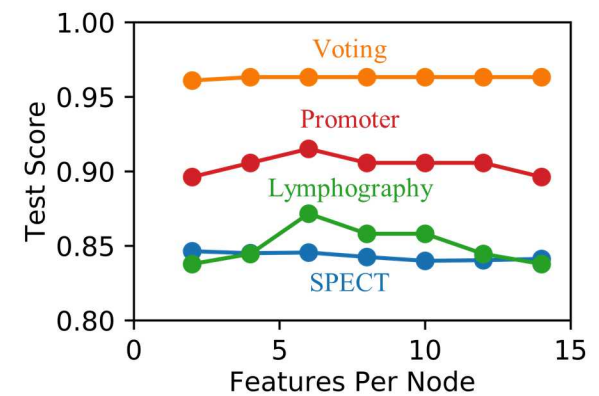
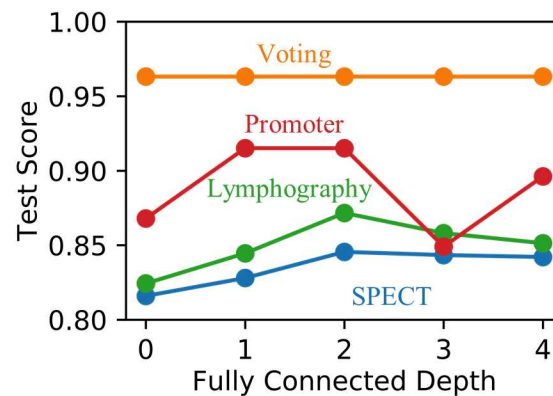
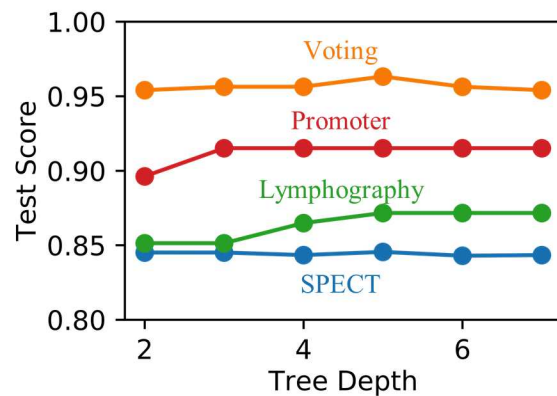
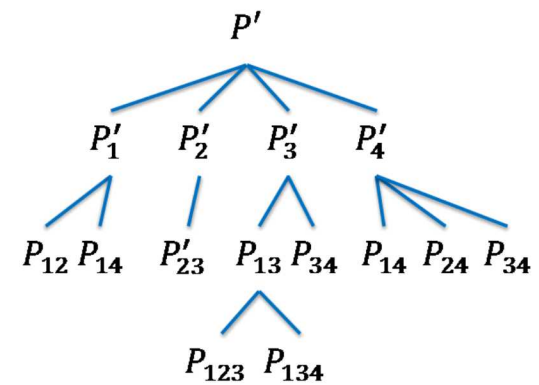
$P_i = P(Y = 1 | x_i = x'_i)$

$P_{ij} = P(Y = 1 | x_i = x'_i, x_j = x'_j)$

$P_{ijk} = P(Y = 1 | x_i = x'_i, x_j = x'_j, x_k = x'_k)$

# Limit Tree Size to Limit Computational Time

- Increasing the tree depth beyond 6 levels does not increase the accuracy on the tested data sets
- Only the first couple layers need to be fully connected
- After that, only the top 6 to 10 features that minimize entropy/gini coefficient need to be kept at each node

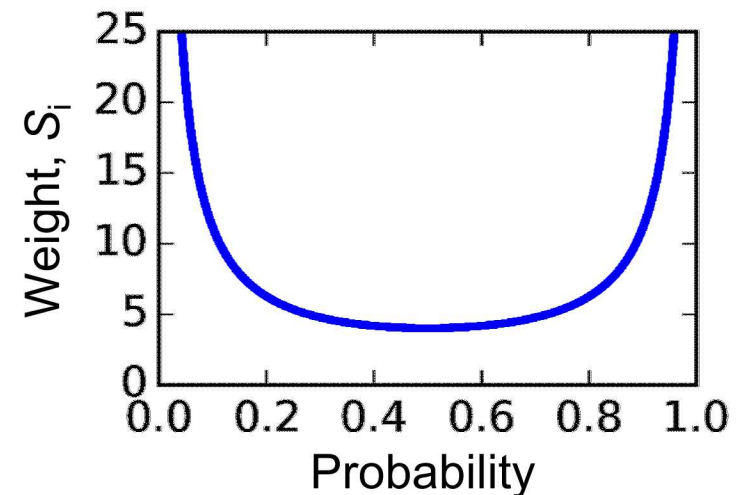


# Weight $P=0$ and $P=1$ More Strongly

Features that predict  $Y'$  more strongly should be weighted more.

$$P' = \frac{\sum_i P'_i \times S_i}{\sum_i S_i}$$

$$S_i = \frac{1}{P'_i \times (1 - P'_i)}$$



Tried logarithmic scaling, but empirically does not work as well

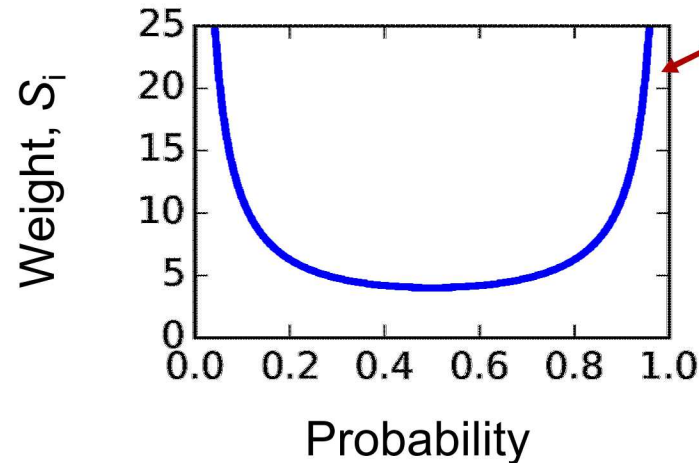
$P = P(Y = 1)$   
 $P_i = P(Y = 1 | x_i = x'_i)$ ,  $P'_i$  = estimate of  $P_i$

$$S_i = \frac{\log(P'_i / (1 - P'_i))}{P'_i - 0.5}$$

# Add Weights for Noise, Class Imbalance and New Information

- Account for noise / limited data counts

- Limit  $S_i$
- Scale  $\sqrt{N_{\text{data}}}$



Need to avoid large weights due to noise, i.e.,  $P_i=1$  based on 1 data point

- Account for class imbalance
- Weight features that give new information / significantly change the estimated probability



# Can Express as a Simple Weighted Average

$$\begin{aligned} P = & \sum_i w_i \times P(Y = 1 | x_i = x_i') + \\ & \sum_{ij} w_{ij} \times P(Y = 1 | x_i = x_i', x_j = x_j') + \\ & \sum_{ijk} w_{ijk} \times P(Y = 1 | x_i = x_i', x_j = x_j', x_k = x_k') + \\ & \dots \end{aligned}$$

Can dynamically update model by updating probabilities.  
Weights are entirely derived from the probabilities

# Fitting the model means optimizing 7 hyperparameters

- nbins: Number of bins for continuous valued data
- TreeDepth, FullyConnectedDepth and FeaturesPerNode
  - Tree creation metaparameters
- $n_{\max}$ ,  $n_{\text{err}}$ : Noise related metaparameters
- UsefulnessModel: usefulness model

# AWE-ML is as accurate as conventional methods



| Dataset        | AWE-ML        | Linear SVM    | SVM (RBF)     | Logistic Regression | Random Forests |
|----------------|---------------|---------------|---------------|---------------------|----------------|
| Bank           | 90.1% ± 0.3%  | 90.1% ± 0.4%  | 89.2% ± 0.1%  | 90.1% ± 0.3%        | 90.4% ± 0.2%   |
| Breast Cancer  | 96.7% ± 1.9%  | 96.5% ± 1.4%  | 96.9% ± 2.5%  | 96.7% ± 2.3%        | 95.1% ± 1.9%   |
| Credit         | 82.2% ± 0.3%  | 79.7% ± 0.6%  | 82.0% ± 0.6%  | 81.1% ± 0.3%        | 81.6% ± 0.4%   |
| Customer       | 92.0% ± 2.3%  | 91.1% ± 2.3%  | 92.5% ± 3.9%  | 90.2% ± 4.9%        | 92.2% ± 2.5%   |
| Iris           | 98.0% ± 3.0%  | 96.0% ± 6.1%  | 96.0% ± 4.4%  | 95.3% ± 5.2%        | 96.0% ± 4.4%   |
| Lymphography   | 85.5% ± 11.9% | 85.1% ± 12.9% | 83.7% ± 10.5% | 83.7% ± 7.8%        | 84.4% ± 3.9%   |
| Promoter       | 94.3% ± 6.4%  | 93.3% ± 6.0%  | 92.4% ± 5.7%  | 92.4% ± 7.0%        | 91.5% ± 10.8%  |
| Spect          | 83.0% ± 6.0%  | 82.0% ± 4.9%  | 79.4% ± 1.3%  | 79.4% ± 1.3%        | 81.2% ± 5.7%   |
| Splice         | 96.4% ± 0.9%  | 95.0% ± 1.2%  | 86.4% ± 1.1%  | 95.9% ± 0.9%        | 94.6% ± 1.1%   |
| Transfusion    | 78.0% ± 2.7%  | 77.1% ± 2.0%  | 76.0% ± 0.3%  | 76.7% ± 2.4%        | 73.1% ± 2.7%   |
| Voting Records | 96.7% ± 1.8%  | 94.4% ± 3.5%  | 95.1% ± 2.1%  | 95.4% ± 3.0%        | 95.1% ± 2.1%   |
| Average        | 90.3%         | 89.1%         | 88.1%         | 88.8%               | 88.65%         |

| Dataset            | AWE-ML       | Random Forests |
|--------------------|--------------|----------------|
| SCOT Alerts        | 96.6% ± 1.3% | 97.4% ± 1.0%   |
| System Call Counts | 94.5% ± 0.7% | 95.0% ± 0.7%*  |

Hyper parameters for all classifiers optimized using 4 fold cross validation

\* System Call Counts Accuracy using binned data with random forests is 94.6%

# Analyze a Misclassified SCOT Instance

**Predicted the alert should be closed with 83% probability**

| Feature 1            | Feature 2      | Counts<br>Closed | Counts<br>Promoted | Probability<br>Closed | Weight |
|----------------------|----------------|------------------|--------------------|-----------------------|--------|
| topic_2 = 1          | time_month = 2 | 2166             | 145                | 94%                   | 2.1%   |
| time_weekday = 0     | time_month = 2 | 1381             | 144                | 91%                   | 1.8%   |
| time_weekday = 0     | topic_2 = 1    | 1149             | 54                 | 96%                   | 1.8%   |
| time_weekday = 0     | topic_3 = 1    | 1667             | 147                | 92%                   | 1.7%   |
| topic_3 = 1          | time_month = 2 | 2817             | 233                | 92%                   | 1.7%   |
| time_weekday = 0     | topic_1 = 1    | 1705             | 143                | 92%                   | 1.7%   |
| topic_1 = 1          | time_month = 2 | 1987             | 147                | 93%                   | 1.7%   |
| time_weekday = 0     | topic_0 = 1    | 1102             | 122                | 90%                   | 1.5%   |
| topic_0 = 1          | time_month = 2 | 1702             | 202                | 89%                   | 1.5%   |
| corr_class_1 = 0     | topic_0 = 1    | 6201             | 226                | 96%                   | 1.3%   |
| splunk_search_97 = 0 | topic_0 = 1    | 6201             | 226                | 96%                   | 1.3%   |

...

- Top feature combinations are dominated by date based features!
  - Not helpful for predicting attacks in the future
- No particular combination of features dominates



# Analyze Individual Features

| Feature                | Weighted Probability | Original Probability | Weight |
|------------------------|----------------------|----------------------|--------|
| time_month = 2         | 83%                  | 97%                  | 10.94% |
| time_weekday = 0       | 82%                  | 97%                  | 10.74% |
| topic_0 = 1            | 76%                  | 96%                  | 8.90%  |
| topic_4 = 9            | 68%                  | 96%                  | 7.87%  |
| time_day = 17          | 57%                  | 88%                  | 7.77%  |
| topic_2 = 1            | 92%                  | 98%                  | 7.71%  |
| topic_3 = 1            | 87%                  | 97%                  | 7.65%  |
| topic_1 = 1            | 86%                  | 98%                  | 7.46%  |
| corr_class_0 = 0       | 92%                  | 99%                  | 5.20%  |
| time_year = 0          | 92%                  | 99%                  | 5.19%  |
| corr_class_unknown = 0 | 92%                  | 99%                  | 5.19%  |
| splunk_search_97 = 0   | 93%                  | 99%                  | 5.19%  |
| corr_class_1 = 0       | 93%                  | 99%                  | 5.13%  |
| corr_class_None = 0    | 94%                  | 99%                  | 5.06%  |

Probability given all feature combinations containing the specified feature

Probability given a single feature



# Eliminate Date Based Features and Analyze a Correctly Classified Instance

| Feature 1                     | Feature 2                | Feature 3   | Count Closed | Counts Promoted | Weight |
|-------------------------------|--------------------------|-------------|--------------|-----------------|--------|
| http_user_agent_perl = 0      |                          |             | 2240         | 0               | 66.5%  |
| http_method_post = 0          | topic_3 = 3              |             | 1508         | 0               | 6.6%   |
| http_method_post = 0          | topic_1 = 2              |             | 917          | 0               | 5.9%   |
| http_method_post = 0          | topic_2 = 2              |             | 1158         | 0               | 5.0%   |
| http_method_post = 0          | topic_0 = 7              |             | 1114         | 0               | 5.0%   |
| http_method_post = 0          | topic_4 = 2              |             | 813          | 0               | 4.5%   |
| http_response_body_length = 4 |                          |             | 1038         | 0               | 3.8%   |
| http_request_body_length = 6  |                          |             | 622          | 0               | 2.2%   |
| topic_1 = 2                   | http_status_code_404 = 0 | topic_3 = 3 | 441          | 0               | 0.3%   |

...

A single feature dominated the classification and we can see why, all 2,240 times it appeared in the training data, the alert was closed

# Analyze another misclassified instance

Incorrectly Predicted the alert should be closed with 99.5% probability

| Feature 1            | Feature 2                | Feature 3   | Feature 4   | Feature 5              | Counts<br>Closed | Counts<br>Promoted | Prob.<br>Closed | Weight |
|----------------------|--------------------------|-------------|-------------|------------------------|------------------|--------------------|-----------------|--------|
| topic_1 = 1          | http_status_code_200 = 0 | topic_4 = 1 | topic_2 = 1 | topic_3 = 1            | 665              | 1                  | 99.8%           | 7.5%   |
| topic_1 = 1          | http_status_code_200 = 0 | topic_4 = 1 | topic_3 = 1 | topic_0 = 8            | 726              | 1                  | 99.9%           | 5.0%   |
| topic_4 = 1          | corr_class_None = 0      |             |             |                        | 3219             | 7                  | 99.8%           | 2.7%   |
| splunk_search_97 = 0 | topic_4 = 1              |             |             |                        | 3219             | 7                  | 99.8%           | 2.7%   |
| corr_class_1 = 0     | topic_4 = 1              |             |             |                        | 3219             | 7                  | 99.8%           | 2.7%   |
| topic_4 = 1          | corr_class_unknown = 0   |             |             |                        | 3219             | 7                  | 99.8%           | 2.7%   |
| corr_class_0 = 0     | topic_4 = 1              |             |             |                        | 3219             | 7                  | 99.8%           | 2.7%   |
| topic_1 = 1          | http_status_code_200 = 0 | topic_4 = 1 | topic_3 = 1 | corr_class_unknown = 0 | 732              | 1                  | 99.9%           | 2.3%   |
| http_method_post = 0 | corr_class_unknown = 0   |             |             |                        | 9133             | 24                 | 99.7%           | 2.1%   |

...

There is always at least one case promoted for every feature combination. Could we create new metrics to find rare events?

# Analyze Misclassified FARM System Call

**Incorrectly Predicted Malware with 78.9% probability**

| Feature 1       | Feature 2           | Feature 3          | Feature 4        | Feature 5        | Feature 6        | Count Good | Count Bad | Weight |
|-----------------|---------------------|--------------------|------------------|------------------|------------------|------------|-----------|--------|
| CreateEvent=1   | FreeVirtMem=1       | OpenSection=2      | SetInfoFile=2    |                  |                  | 0          | 3         | 8.4%   |
| CreateEvent=1   | QryDirFile=0        | QrySysInfo=1       | SetInfoThread=1  | UnmapViewOfSec=4 | UsrRegWindMsg= 1 | 84         | 0         | 6.6%   |
| CreateEvent=1   | QryDirFile=0        | QryInfoFile=4      | QrySysInfo=1     | SetInfoThread=1  | UsrRegWindMsg=1  | 50         | 0         | 4.1%   |
| CreateSection=4 | QryAttributesFile=4 | RqstWaitReplyPrt=4 | WaitForMultObj=1 |                  |                  | 0          | 283       | 4.1%   |
| CreateThread=0  | OpenSection=2       | QrySection=3       | SetInfoFile=2    | UsrRegWindMsg=1  |                  | 0          | 25        | 3.2%   |
| OpenSection=2   | ReadFile=3          | SetInfoFile=2      | SysCall#240=0    | SysCall#326=0    |                  | 0          | 8         | 2.9%   |
| OpenSection=2   | ReadFile=3          | SetInfoFile=2      | SysCall#240=0    | SysCall#264=0    |                  | 0          | 8         | 2.6%   |
| CreateEvent=1   | QryDefaultLocale=1  | QryInfoJobObj=0    | QryKey=0         | SysCall#92=1     | SetInfoFile=2    | 0          | 5         | 2.5%   |
| OpenSection=2   | OpenThreadTkn=1     | QryInfoJobObj=0    | SetInfoFile=2    | SysCall#172=0    |                  | 0          | 2         | 2.5%   |
| CreateFile=3    | CreateSection=4     | RqstWaitReplyPrt=4 | WaitForOneObj=0  |                  |                  | 0          | 5         | 2.4%   |
| FreeVirtMem=1   | FsControlFile=2     | RqstWaitReplyPrt=4 | SysCall#249=1    |                  |                  | 0          | 8         | 2.3%   |

...

There is contradictory information resulting in the misclassification

# Summary

- Matches state of the art machine learning accuracy
  - Identical on open datasets, within 1% on cyber datasets
- Fully explainable
- Coded in Cython for speed
- Compatible with Sci-kit Learn
- To do:
  - Further improve accuracy, automate meta parameter settings
  - Simplify explanations
  - Handle continuous valued data
  - Parallelize code
  - Adapt to new data without retraining
  - Extend to Regression

$$P = \sum_i w_i \times P(Y = 1 | x_i = x_i') + \\ \sum_{ij} w_{ij} \times P(Y = 1 | x_i = x_i', x_j = x_j') + \\ \dots$$

# Backup/Extra Slides



# Lets look at the importance by feature

## Incorrectly Predicted Malware with 78.9% probability

| Feature                         | Weighted Probability | Original Probability | Weight |
|---------------------------------|----------------------|----------------------|--------|
| NtSetInformationFile = 2        | 96.7%                | 19.7%                | 11.1%  |
| NtOpenSection = 2               | 99.8%                | 27.4%                | 8.4%   |
| NtCreateEvent = 1               | 60.4%                | 29.7%                | 5.3%   |
| NtReadFile = 3                  | 95.3%                | 20.6%                | 3.9%   |
| NtFreeVirtualMemory = 1         | 96.6%                | 48.6%                | 3.9%   |
| NtUserRegisterWindowMessage = 1 | 46.2%                | 16.5%                | 3.7%   |
| NtSetInfoThread = 1             | 47.9%                | 27.4%                | 3.6%   |
| NtRequestWaitReplyPort = 4      | 99.3%                | 76.2%                | 3.2%   |
| NtQueryDirectoryFile = 0        | 35.5%                | 43.0%                | 2.9%   |
| NtFsControlFile = 2             | 91.1%                | 21.7%                | 2.9%   |
| NtQuerySystemInformation = 1    | 3.8%                 | 26.7%                | 2.0%   |
| NtOpenThreadToken = 1           | 98.0%                | 31.2%                | 1.9%   |
| NtCreateSection = 4             | 95.1%                | 67.8%                | 1.9%   |
| NtQueryInformationFile = 4      | 54.1%                | 22.1%                | 1.8%   |
| NtUnmapViewOfSec = 4            | 31.5%                | 34.0%                | 1.7%   |
| NtCreateFile = 3                | 67.1%                | 22.3%                | 1.6%   |
| SysCall#326 = 0                 | 86.3%                | 65.1%                | 1.6%   |
| NtMapViewOfSec = 3              | 69.5%                | 32.3%                | 1.6%   |
| SysCall#240 = 0                 | 98.0%                | 39.7%                | 1.5%   |

...

Probability given all feature combinations containing the specified feature

Top 20 most important of 384 features

May be able to map the key system calls back to the part of the file that is malware

Accounting for feature combinations significantly changes the probability

# Analyze Correctly Classified FARM System Call

**Correctly Predicted Malware with 99.9998% probability**

| Feature 1            | Feature 2       | Feature 3       | Feature 4        | Feature 5          | Feature 6           | Count Good | Count Bad | Weight |
|----------------------|-----------------|-----------------|------------------|--------------------|---------------------|------------|-----------|--------|
| FsControlFile=4      | MapViewOfSec=4  | OpenProcTokn=1  | QryAttribFile=4  | SetInfoProcess=4   | WaitForMultObj=0    | 0          | 288       | 13.1%  |
| MapViewOfSec=4       | OpenKey=4       | SysCall#92=1    | SetInfoThread=2  | WaitForOneObj=3    |                     | 0          | 169       | 3.8%   |
| OpenKey=4            | OpenSection=3   | SysCall#92=1    | SetInfoThread=2  |                    |                     | 0          | 133       | 3.8%   |
| CreateFile=4         | CreateMutant=3  | FsControlFile=4 | MapViewOfSec=4   | UnmapViewOfSec=4   | WaitForMultObj=0    | 0          | 125       | 3.4%   |
| FlushInstructCache=1 | FsControlFile=4 | MapViewOfSec=4  | QryAttribFile=4  | WaitForOneObj=3    |                     | 0          | 334       | 2.7%   |
| SysCall#0=0          | AccessCheck=0   | CreateSection=4 | SetInfoThread=2  |                    |                     | 0          | 315       | 2.5%   |
| CreateSection=4      | OpenProcTokn=1  | SetInfoThread=2 | UnmapViewOfSec=4 | WaitForMultObj=0   | UsrValidateSecure=0 | 0          | 216       | 2.5%   |
| CreateSection=4      | OpenDirObject=2 | OpenProcTokn=1  | SetInfoThread=2  | WaitForMultObj=0   | UsrValidateSecure=0 | 0          | 219       | 2.3%   |
| SysCall#0=0          | CreateSection=4 | SetInfoThread=2 | WaitForOneObj=3  | UserSysParamInfo=0 |                     | 0          | 333       | 2.2%   |
| CreateFile=4         | MapViewOfSec=4  | QueryValueKey=4 | WriteVirtMem=0   |                    |                     | 0          | 328       | 1.9%   |
| MapViewOfSec=4       | OpenKey=4       | SysCall#92=1    | SetInfoThread=2  | WaitForMultObj=0   |                     | 0          | 79        | 1.8%   |

# By Feature

**Correctly Predicted Malware with 99.9998% probability**

| Feature                        | Weighted Probability | Original Probability | Weight |
|--------------------------------|----------------------|----------------------|--------|
| NtMapViewOfSection = 4         | 100.0%               | 82.3%                | 8.8%   |
| NtWaitForMultipleObjects = 0   | 100.0%               | 37.4%                | 8.1%   |
| NtFsControlFile = 4            | 100.0%               | 66.6%                | 7.2%   |
| NtSetInformationThread = 2     | 100.0%               | 88.5%                | 7.2%   |
| NtWaitForSingleObject = 3      | 100.0%               | 40.8%                | 5.2%   |
| NtOpenKey = 4                  | 100.0%               | 51.4%                | 5.1%   |
| NtOpenProcessToken = 1         | 100.0%               | 34.4%                | 4.4%   |
| NtQueryAttributesFile = 4      | 100.0%               | 55.3%                | 3.4%   |
| SysCall#92 = 1                 | 100.0%               | 32.0%                | 3.2%   |
| NtSetInformationProcess = 4    | 100.0%               | 59.9%                | 3.2%   |
| NtCreateSection = 4            | 100.0%               | 67.8%                | 2.7%   |
| NtCreateFile = 4               | 100.0%               | 28.5%                | 2.4%   |
| NtQuerySection = 4             | 100.0%               | 78.3%                | 2.1%   |
| NtUserSystemParametersInfo = 0 | 100.0%               | 71.0%                | 2.0%   |
| NtUnmapViewOfSection = 4       | 100.0%               | 34.0%                | 1.8%   |
| NtCreateEvent = 4              | 100.0%               | 72.4%                | 1.6%   |
| SysCall#0 = 0                  | 100.0%               | 29.5%                | 1.4%   |
| NtOpenSection = 3              | 100.0%               | 44.0%                | 1.4%   |
| NtOpenDirectoryObject = 2      | 100.0%               | 49.8%                | 1.3%   |

Top 20 most important of 384 features

...

Probability given all feature combinations containing the specified feature

Probability given a single feature



# Use Model to Analyze a Misclassified Result

## 1984 Congressional Voting Records Dataset

The classifier predicted with 70% probability that this Member of Congress would be a Republican when they are a Democrat.

| Features   | Counts Rep. | Counts Dem. | Probability Rep. | Weight | Cumulative Weight |
|--|-------------|-------------|------------------|--------|-------------------|
| Immigration-Y, South Africa Export Act-N             | 16          | 0           | 100%             | 19.4%  | 19.4%             |
| Doc Fee-Y, Mx Missile-N, Immigration-Y, Duty Free-N  | 47          | 0           | 100%             | 4.8%   | 24.2%             |
| Doc Fee-Y, Contras aid-N, Immigration-Y, Duty Free-N | 47          | 0           | 100%             | 4.7%   | 28.9%             |
| Adopt Budget-Y, Synfuels cutback-Y, Education-N      | 0           | 58          | 0%               | 4.0%   | 32.9%             |
| Water-Y, Adopt Budget-Y, Synfuels cutback-Y,         | 0           | 38          | 0%               | 3.1%   | 36.0%             |

| Feature #                       | Probability Republican | Weight | Feature #                     | Probability Republican | Weight |
|---------------------------------|------------------------|--------|-------------------------------|------------------------|--------|
| Immigration-Y                   | 95%                    | 17%    | Mx missile-N                  | 86%                    | 4%     |
| Doc fee freeze-Y                | 94%                    | 16%    | Nicaraguan contra aid – N     | 83%                    | 4%     |
| South Africa Export Admin Act-N | 94%                    | 14%    | Anti-satellite test ban-N     | 29%                    | 3%     |
| Adopt Budget-Y                  | 14%                    | 8%     | Handicapped infants-N         | 78%                    | 3%     |
| Synfuels corporation cutback-Y  | 23%                    | 8%     | Crime-Y                       | 55%                    | 2%     |
| Education spending-N            | 21%                    | 6%     | El Salvador aid-Y             | 69%                    | 2%     |
| Duty free exports-N             | 89%                    | 5%     | Superfund right to sue-Y      | 52%                    | 2%     |
| Water project cost sharing-Y    | 53%                    | 4%     | Religious groups in schools-Y | 56%                    | 2%     |

Republican features have higher certainty and therefore higher weight

Probability given all feature combinations containing the specified feature

# Analyze a Correctly Classified Result

## 1984 Congressional Voting Records Dataset

The classifier correctly predicted this member of congress is a republican

| Features  | Counts Rep. | Counts Dem. | Probability Rep. | Weight | Cumulative Weight |
|---|-------------|-------------|------------------|--------|-------------------|
| Budget -N, Doc Fee-Y, Immigration-Y                       | 54          | 0           | 100%             | 18.3%  | 18.3%             |
| Doc Fee-Y, Immigration-Y, Education -Y                    | 57          | 0           | 100%             | 16.1%  | 34.4%             |
| Immigration-Y, Education-Y, SA Export-N                   | 16          | 0           | 100%             | 5.0%   | 39.4%             |
| Water-N, Doc Fee-Y, Immigration-Y                         | 31          | 0           | 100%             | 3.0%   | 42.4%             |
| Water-N, Immigration-Y, SA Export-N                       | 6           | 0           | 100%             | 0.9%   | 43.3%             |
| Handicap-N, Budget-N, Doc Fee-Y, MxMissile-N, Superfund-Y | 76          | 1           | 98.7%            | 0.5%   | 43.8%             |



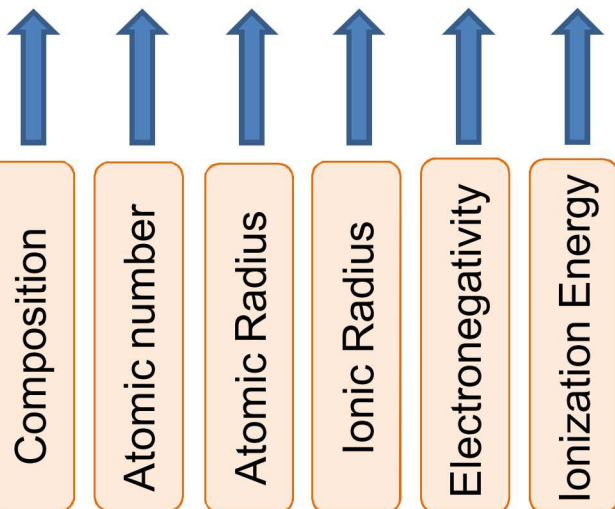
# Conventional vs explainable machine learning

## Conventional ML

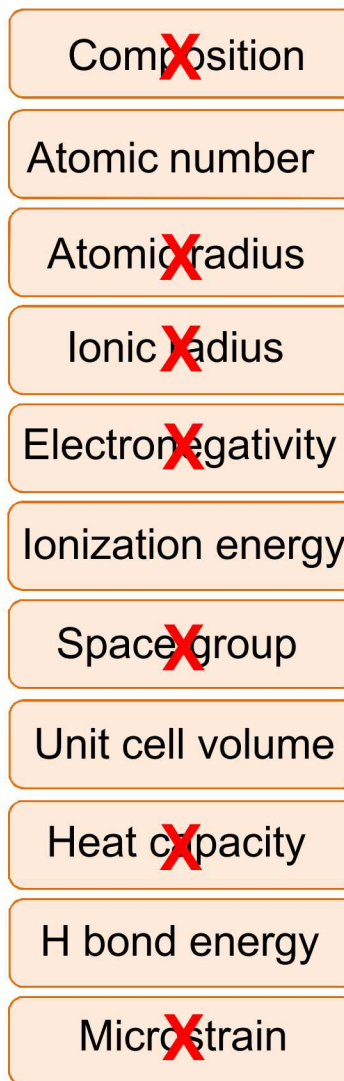
Observable: *Metal reacts with  $H_2$  at SPT*



Black Box



...



## Explainable ML

Observable: *Metal reacts with  $H_2$  at SPT*



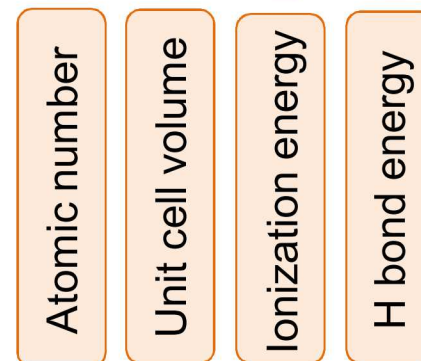
Contribution  
(average weight)

15%

20%

25%

40%

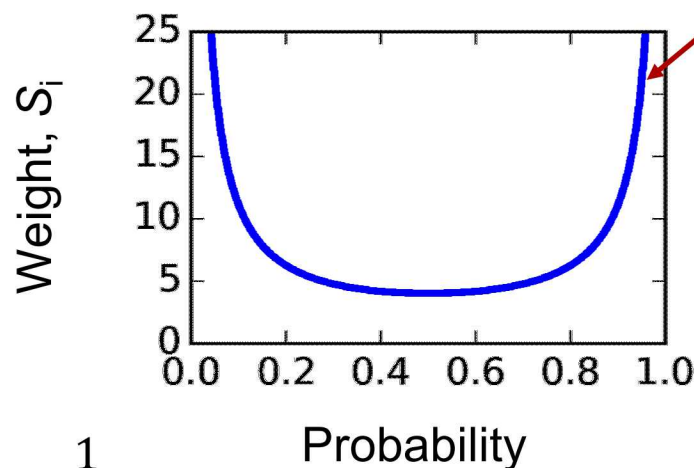


AWE-ML

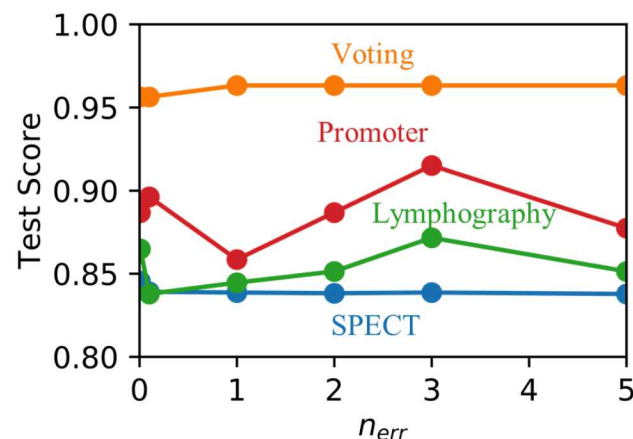
⇒ *The EML framework has the potential to address exceedingly complex interrelationships among features that defy scientific intuition to extract structure-property relationships*

# Account for Noise: Regularization

- Each probability estimate,  $P_i$ ,  $P_{ij}$ , etc is backed by some number of training examples,  $n$ .
  - Limit  $P=0/1$  scaling based on  $n$ .
    - Limit  $P_i$  used to calculate  $S_i$  to  $\left[\frac{n_{err}}{n}, 1 - \frac{n_{err}}{n}\right]$ 
      - $n_{err}$  is a meta-parameter around 1, represents average number of examples that might be wrong due to noise
      - If  $n < n_{err}$ , set  $P_i = 0.5$
- Need to avoid large weights due to noise, i.e.,  $P_i = 1$  based on 1 data point



$$S_i = \frac{1}{P'_i \times (1 - P'_i)}$$



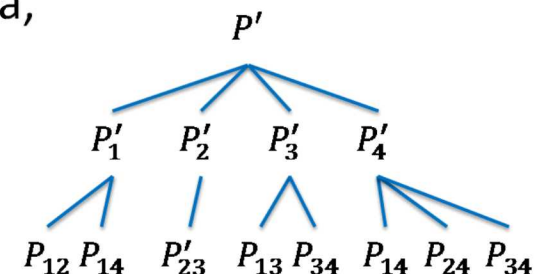
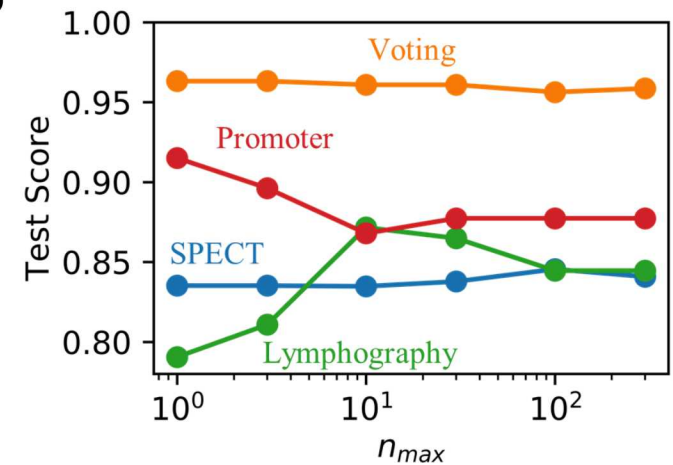
# Additionally add a weight based on the number of samples

- Each probability estimate,  $P_i$ ,  $P_{ij}$ , etc is backed by a some number of training examples,  $n$ .
- Determine a weight based on  $n$ 
  - Define  $n_{\max}$  = # of training examples to needed to overcome noise
  - Scaling factor =  $N_i = \min(\sqrt{n_i}, \sqrt{n_{\max}})$
  - Noise tends to scale with variance, proportional to sqrt (N)

$$P' = \frac{\sum_i P'_i \times S_i \times N_i}{\sum_i S_i \times N_i}$$

- If none of the probabilities are backed by significant data, use the parent probability:

$$P' = \frac{\max_i(N_i)}{N} \times \frac{\sum_i P'_i \times S_i \times N_i}{\sum_i S_i \times N_i} + \left(1 - \frac{\max_i(N_i)}{N}\right) \times P$$



# Account For Class Imbalance

- Allow rare classes to have larger weights to compensate for lower counts

Previously

Limit  $P_i$  used to calculate  $S_i$  to  $\left[\frac{n_{err}}{n}, 1 - \frac{n_{err}}{n}\right]$

Multiply by  $1 - P(Y = Y')$

Multiply by  $P(Y = Y')$

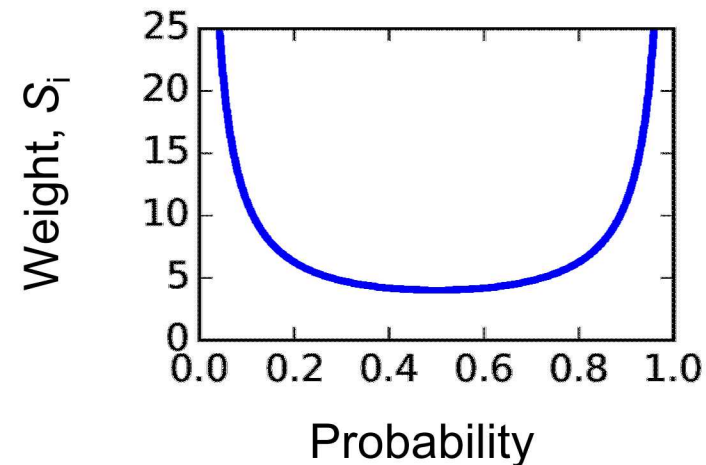
$$P' = \frac{\sum_i P'_i \times S_i}{\sum_i S_i}$$

$$S_i = \frac{1}{P'_i \times (1 - P'_i)}$$

Now

$$P_{i,max} = \max\left(1 - \left(P(Y = Y') \frac{n_{err}}{n}\right), 0.5\right)$$

$$P_{i,min} = \min\left(\left(1 - P(Y = Y')\right) \times \frac{n_{err}}{n}, 0.5\right)$$



# Add a weight based on usefulness of a feature

- Estimate usefulness by how much each feature changes the probability around the decision function. Three possible models for usefulness are:

**None**

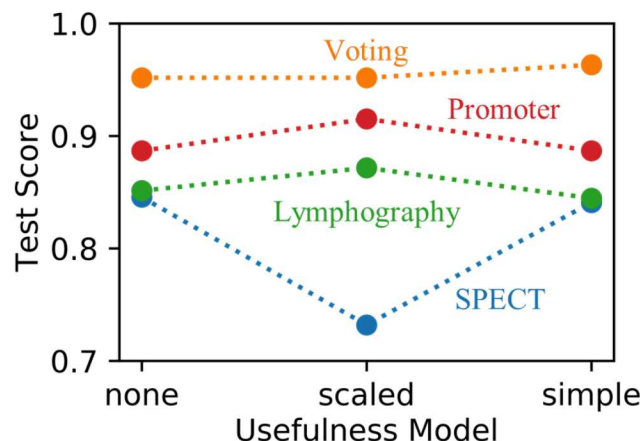
$$U_i = 1$$

**Simple**

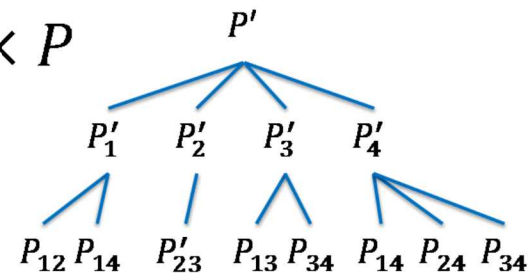
$$U_i = \frac{P'_i - P}{P'_i + P}$$

**Scaled**

$$U_i = |S_i \times (P'_i - 0.5) - S_o \times (P - 0.5)|$$



$$P' = \frac{\max(N_i)}{N} \times \frac{\sum_i P'_i \times S_i \times N_i \times U_i}{\sum_i S_i \times N_i \times U_i} + \left(1 - \frac{\max(N_i)}{N}\right) \times P$$





# Thus the overall model is:

$$P' = \frac{\max_i(N_i)}{N} \times \frac{\sum_i P'_i \times S_i \times N_i \times U_i}{\sum_i S_i \times N_i \times U_i} + \left(1 - \frac{\max_i(N_i)}{N}\right) \times P$$

$$P'_i = \frac{\max_j(N_{ij})}{N_i} \times \frac{\sum_{j \neq i} P'_{ij} \times S_{ij} \times N_{ij} \times U_{ij}}{\sum_{j \neq i} S_{ij} \times N_{ij} \times U_{ij}} + \left(1 - \frac{\max_j(N_{ij})}{N_i}\right) \times P_i$$

$$P'_{ij} = \frac{\max_k(N_{ijk})}{N_{ij}} \times \frac{\sum_{k \neq j \neq i} P'_{ijk} \times S_{ijk} \times N_{ijk} \times U_{ijk}}{\sum_{k \neq j \neq i} S_{ijk} \times N_{ijk} \times U_{ijk}} + \left(1 - \frac{\max_k(N_{ijk})}{N_{ij}}\right) \times P_{ij}$$

Where:

$$P = P(Y = 1)$$

$$P_i = P(Y = 1 | x_i = x'_i)$$

$$P_{ij} = P(Y = 1 | x_i = x'_i, x_j = x'_j)$$

$$P_{ijk} = P(Y = 1 | x_i = x'_i, x_j = x'_j, x_k = x'_k)$$

$$S_i = \frac{1}{P'_i \times (1 - P'_i)}$$

$$U_i = \frac{P'_i - P}{P'_i + P}$$

$$N_i = \min(\sqrt{n_i}, \sqrt{n_{max}})$$