COMP 551 - Applied Machine Learning Lecture 10 — Ensemble methods

William L. Hamilton

(with slides and content from Joelle Pineau)

Multiclass Bernoulli Naïve Bayes'

Key idea of Naïve Bayes' :

Marginal probability of class k

Probability of the observed features given class k

$$P(y = k|\mathbf{x}) \propto P(y = k)P(\mathbf{x}|y)$$

Probability that data point is from class k

$$= P(y = k)\prod_{j=1}^{m} P(x_j|y)$$

Assume features are independent (**Naïve Bayes' assumption**)

Take logarithm for numerical stability

$$\propto \log(P(y = k)) + \sum_{j=1}^{m} \log(P(x_j|y))$$

Multiclass Bernoulli Naïve Bayes

- For **Bernoulli** Naïve Bayes, we assume that the features x_j are binary.

- What are the parameters? We need to learn:

Marginal probability for each class. (Note that we only need to learn the parameter for K-1 classes, since the probability for the Kth class can then be inferred)

$$\theta_k = P(y = k) \qquad k = 1, 2, ..., K - 1$$

Conditional probability of each feature given each class. In other words, how often is feature j equal to 1 for points from class k?

$$\theta_{j,k} = P(x_j = 1 | y = k) \qquad k = 1, 2, ..., K$$

Multiclass Bernoulli Naïve Bayes

In other words:

$$\theta_k = P(y=k)$$
$$= (\#\text{ of examples where } y=1) / (\text{total } \#\text{ of examples})$$

$$\theta_{j,k} = P(x=1 \mid y=k)$$
$$= (\#\text{ of examples where } x_j=1 \text{ and } y=k) / (\#\text{ of examples where } y=k)$$

Multiclass Bernoulli Naïve Bayes

- Practically speaking, how do we compute these parameters?
- Suppose you use the preprocessing class (or something equivalent): sklearn.feature_extraction.text.CountVectorizer with binary=True
  - If you run this on your training data input, then you get a sparse matrix (i.e., scipy.sparse.csr_matrix), $\mathbf{X}$, where every row is a training example and every column corresponds to a binary word feature.
  - $\mathbf{X}_{i,j} = 1$ if word j feature occurs in document/example i; otherwise, $\mathbf{X}_{i,j} = 0$
- Now, using matrix $\mathbf{X}$ and the array $\mathbf{y}$ containing the class labels, compute:

```
theta_k = (y == k).sum() / float(y.shape[0])
theta_j_k = X[y==k][j].sum() / float( (y ==k).sum())
```

- *You should write a for-loop (or equivalent) to do this for all features/classes!

Multiclass Bernoulli Naïve Bayes

How to make predictions?

From Slide 2

$$P(y=k|\mathbf{x}) \propto P(y=k)P(\mathbf{x}|y)$$

$$= P(y=k)\prod_{j=1}^{m} P(x_j|y)$$

$$\propto \log(P(y=k)) + \sum_{j=1}^{m} \log(P(x_j|y))$$

$$= \log(\theta_k) + \sum_{j=1}^{m} x_j \log(\theta_{j,k}) + (1-x_j)\log(1-\theta_{j,k})$$

Rewriting the log probabilities using our parameter notation.

Note that

$$x_j \log(\theta_{j,k}) + (1-x_j)\log(1-\theta_{j,k})$$

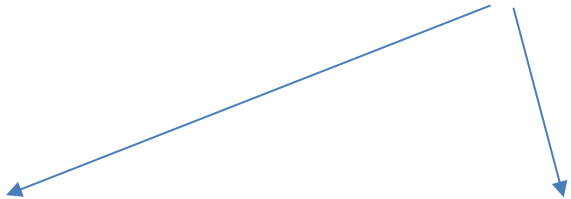
$$= \begin{cases} \log(\theta_{j,k}) = \log(P(x_j=1|y=k)) & \text{if } x_j = 1 \\ \log(1-\theta_{j,k}) = \log(P(x_j=0|y=k)) & \text{if } x_j = 0 \end{cases}$$

Multiclass Bernoulli Naïve Bayes

- Practically speaking, how do we make predictions?
- Given a testing point x (as a numpy array)

```
class_prob = []
for k in range(num_classes)
    feature_likelihood = 0
    for j in range(num_features):
        feature_likelihood += x[j]*np.log(theta[k][j]) + (1-x[j])*np.log(1-theta[k][j])
    class_prob = feature_likelihood + np.log(theta[k])
return np.argmax(class_prob)
```

Assuming that the theta parameters are stored in a dictionary indexed by class index k and feature index j.



- *This is just Python-esque pseudo-code, and there are more efficient ways to implement this (e.g., using vector operations instead of for loops)!

Next topic: Ensemble methods

- Recently seen supervised learning methods:
  - Logistic regression, Naïve Bayes, LDA/QDA
  - Decision trees, Instance-based learning

- Now we will discuss the idea of how we can combine the output of different models, an idea called **ensembling.**

Ensemble learning in general

- Key idea: Run base learning algorithm(s) multiple times, then combine the predictions of the different learners to get a final prediction.
  - What's a base learning algorithm? Naïve Bayes, LDA, Decision trees, SVMs, …

- Option 1 (Bagging): Construct K independent models by training the same base learning algorithm on different subsets of the training data.
- Option 2 (Boosting): Incrementally train K models, where each successive model tries to fix the mistakes of the previous models.

- Option 3 (Stacking): Train K different models and combine their output using a "meta-classifier".

Ensemble learning in general

- Key idea: Run base learning algorithm(s) multiple times, then combine the predictions of the different learners to get a final prediction.
  - What's a base learning algorithm? Naïve Bayes, LDA, Decision trees, SVMs, …

- Option 1 (Bagging): Construct K independent models by training the same base learning algorithm on different subsets of the training data.
- Option 2 (Boosting): Incrementally train K models, where each successive model tries to fix the mistakes of the previous models.

Generally assume that the same base learning algorithm is used to construct all models in the ensemble.

- Option 3 (Stacking): Train K different models and combine their output using a "meta-classifier".

Bootstrapping

- Given dataset D, construct a bootstrap replicate of D, called D_k, which has the same number of examples, by drawing samples from D with replacement.

- Use the learning algorithm to construct a hypothesis h_k by training on D_k.
- Compute the prediction of h_k on each of the remaining points, from the set $T_k = D - D_k$.
- Repeat this process B times, where B is typically a few hundred.

- Similar to cross-validation but using random sampling with replacement.

Estimating bias and variance

- In general, bootstrapping is useful for computing sound statistical estimates of the bias and variance for our model.

- For each point $\mathbf{x}$, we have a set of estimates $\mathrm{h}_1(\mathbf{x}), \ldots, \mathrm{h}_K(\mathbf{x})$, with $K \leq B$ (since $\mathbf{x}$ might not appear in some replicates).
- The average empirical prediction of $\mathbf{x}$ is: $\hat{\mathrm{h}}(\mathbf{x}) = (1/K) \sum_{k=1:K} \mathrm{h}_k(\mathrm{x})$.
- We estimate the bias as: $\mathrm{y} - \hat{\mathrm{h}}(\mathbf{x})$.
- We estimate the variance as: $(1/(K-1)) \sum_{k=1:K} (\hat{\mathrm{h}}(\mathbf{x}) - \mathrm{h}_k(\mathbf{x}))^2$.

Bagging: Bootstrap aggregation

- If we did all the work to get the hypotheses h_k, why not use all of them to make a prediction? (as opposed to just estimating bias/variance/error).

- All hypotheses get to have a vote.
  - For classification: pick the majority class.
  - For regression, average all the predictions.

- Which hypotheses classes would benefit most from this approach?

Bagging

- For each point $\mathbf{x}$, we have a set of estimates $h_1(\mathbf{x}), \ldots, h_K(\mathbf{x})$, with $K \leq B$ (since $\mathbf{x}$ might not appear in some replicates).
  - The average empirical prediction of $\mathbf{x}$ is: $\hat{h}(\mathbf{x}) = (1/K) \sum_{k=1:K} h_k(x)$.
  - We estimate the bias as: $y - \hat{h}(\mathbf{x})$.
  - We estimate the variance as: $(1/(K-1)) \sum_{k=1:K} (\hat{h}(\mathbf{x}) - h_k(\mathbf{x}))^2$.

Bagging

- For each point $\mathbf{x}$, we have a set of estimates $h_1(\mathbf{x}), \ldots, h_K(\mathbf{x})$, with $K \leq B$ (since $\mathbf{x}$ might not appear in some replicates).
  - The average empirical prediction of $\mathbf{x}$ is: $\hat{h}(\mathbf{x}) = (1/K) \sum_{k=1:K} h_k(x)$.
  - We estimate the bias as: $y - \hat{h}(\mathbf{x})$.
  - We estimate the variance as: $(1/(K-1)) \sum_{k=1:K} (\hat{h}(\mathbf{x}) - h_k(\mathbf{x}))^2$.

- In theory, bagging eliminates variance altogether.
- In practice, bagging tends to reduce variance and increase bias.
- Use this with "unstable" learners that have high variance, e.g., decision trees or nearest-neighbours.

Random forests (Breiman)

- Basic algorithm:
  - Use K bootstrap replicates to train K different trees.
  - At each node, pick m variables at random (use $m<M$, the total number of features).
  - Determine the best test (using normalized information gain).
  - Recurse until the tree reaches maximum depth (no pruning).

Random forests (Breiman)

- Basic algorithm:
  - Use K bootstrap replicates to train K different trees.
  - At each node, pick m features at random (use $m<M$, the total number of features).
  - Determine the best test (using normalized information gain).
  - Recurse until the tree reaches maximum depth (no pruning).

- Comments:
  - Each tree has high variance, but the ensemble uses averaging, which reduces variance.
  - Random forests are very competitive in both classification and regression, but still subject to overfitting.

Extremely randomized trees
(Geurts et al., 2005)

- Basic algorithm:
  - Construct K decision trees.
  - Pick m features at random (without replacement) and pick a random test involving each attribute.
  - Evaluate all tests (using a normalized information gain metric) and pick the best one for the node.
  - Continue until a desired depth or a desired number of instances (n_{min}) at the leaf is reached.

Extremely randomized trees
(Geurts et al., 2005)

- Basic algorithm:
  - Construct K decision trees.
  - Pick m attributes at random (without replacement) and pick a random test involving each attribute.
  - Evaluate all tests (using a normalized information gain metric) and pick the best one for the node.
  - Continue until a desired depth or a desired number of instances (n_{min}) at the leaf is reached.
- Comments:
  - Very reliable method for both classification and regression.
  - The smaller m is, the more randomized the trees are; small m is best, especially with large levels of noise. Small n_{min} means less bias and more variance, but variance is controlled by averaging over trees.

Randomization in general

- Instead of searching very hard for the best hypothesis, generate lots of random ones, then average their results.
- Examples: Random feature selection, random projections of continuous data, …
- Advantages?

- Disadvantages?

Randomization in general

- Instead of searching very hard for the best hypothesis, generate lots of random ones, then average their results.
- Examples: Random feature selection, random projections of continuous data, …
- Advantages?
  - Very fast, easy, can handle lots of data.
  - Can circumvent difficulties in optimization.
  - Averaging reduces the variance introduced by randomization.
- Disadvantages?

Randomization in general

- Instead of searching very hard for the best hypothesis, generate lots of random ones, then average their results.
- Examples: Random feature selection, random projections of continuous data, …
- Advantages?
  - Very fast, easy, can handle lots of data.
  - Can circumvent difficulties in optimization.
  - Averaging reduces the variance introduced by randomization.
- Disadvantages?
  - New prediction may be more expensive to evaluate (go over all trees).
  - Still typically subject to overfitting.
  - Low interpretability (e.g., compared to standard decision trees).

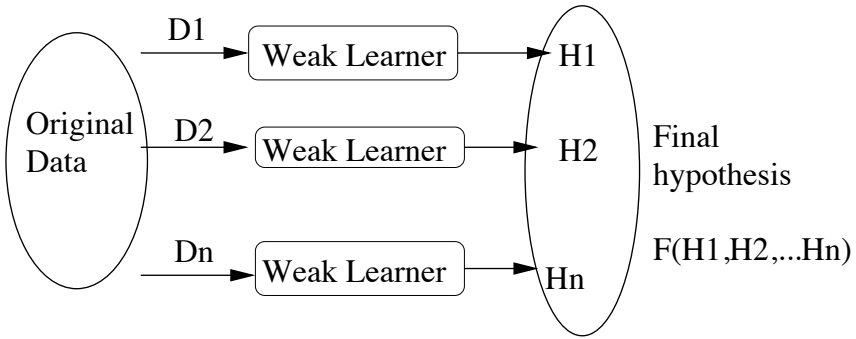
Incrementally constructing an ensemble

- In an ensemble, the output on any instance is computed by combining the outputs of several hypotheses.

- **Idea**: Don't construct the hypotheses independently. Instead, new hypotheses should focus on instances that are problematic for existing hypotheses.
  - If an example is difficult, more components should focus on it.

Boosting

- Basic algorithm:
  - Use the training set to train a simple predictor.
  - Re-weight the training examples, putting more weight on examples that were not properly classified in the previous predictor.
  - Repeat n times.
  - Combine the simple hypotheses into a single, accurate predictor.



Notation

- Assume that examples are drawn independently from some probability distribution P on the set of possible data D.

- Let $\mathrm{J_P(h)}$ be the expected error of hypothesis h when data is drawn from P:

$$\mathrm{J_P(h)} = \sum_{<\mathbf{x},y> \epsilon\, \mathrm{D}} \mathrm{J(h(\mathbf{x}),y)P(<\mathbf{x},y>)}$$

where $\mathrm{J(h(\mathbf{x}),y)}$ could be the squared error, or 0/1 loss.

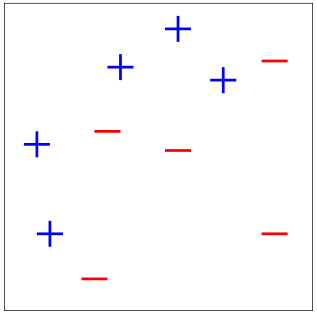
Weak learners

- Assume we have some "weak" binary classifiers:
  - A decision stump is a single node decision tree: $x_i > t$
  - A single feature Naïve Bayes classifier.
  - A 1-nearest neighbour classifier.

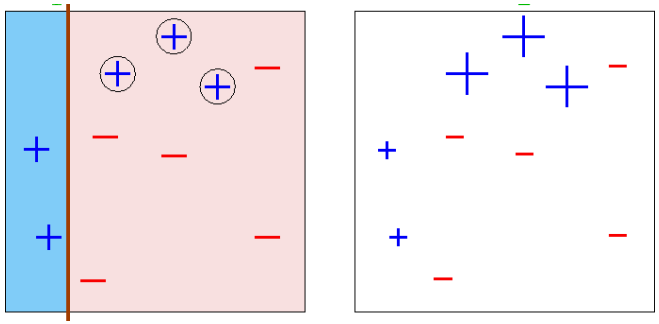
- "Weak" means $J_P(h) < 1/2 - \gamma$ (assuming 2 classes), where $\gamma > 0$
  - So true error of the classifier is only slightly better than random.

- Questions:
  - How do we re-weight the examples?
  - How do we combine many simple predictors into a single classifier?

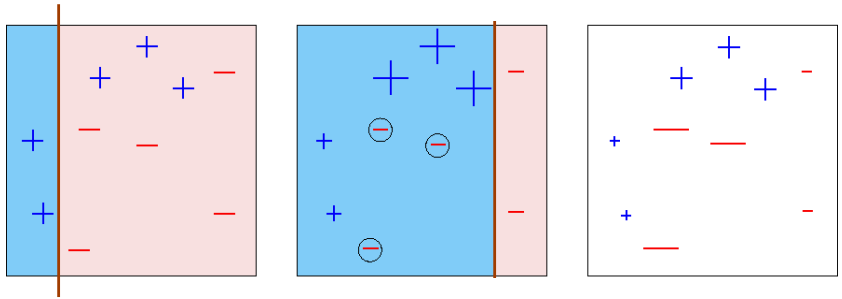
Example



Example: First step



Example: Second step



AdaBoost (Freund & Schapire, 1995)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

AdaBoost (Freund & Schapire, 1995)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : X \to \{-1, +1\}$ with error

$$\epsilon_t = \Pr_{i \sim D_t} \left[h_t(x_i) \neq y_i \right].$$

AdaBoost (Freund & Schapire, 1995)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : X \to \{-1, +1\}$ with error

$$\epsilon_t = \Pr_{i \sim D_t} \left[h_t(x_i) \neq y_i \right].$$

- Choose $\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$. weight of weak learner *t*

AdaBoost (Freund & Schapire, 1995)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : X \to \{-1, +1\}$ with error

$$\epsilon_t = \Pr_{i \sim D_t} \left[h_t(x_i) \neq y_i \right].$$

- Choose $\alpha_t = \frac{1}{2} \ln \left(\frac{1 - \epsilon_t}{\epsilon_t} \right)$. weight of weak learner *t*
- Update:

$$\begin{aligned} D_{t+1}(i) &= \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases} \\ &= \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t} \end{aligned}$$

where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

AdaBoost (Freund & Schapire, 1995)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in X, y_i \in Y = \{-1, +1\}$
Initialize $D_1(i) = 1/m$.
For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t.
- Get weak hypothesis $h_t : X \to \{-1, +1\}$ with error

$$\epsilon_t = \Pr_{i \sim D_t}\left[h_t(x_i) \neq y_i\right].$$

- Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1 - \epsilon_t}{\epsilon_t}\right)$. weight of weak learner *t*
- Update:

$$\begin{aligned} D_{t+1}(i) &= \frac{D_t(i)}{Z_t} \times \begin{cases} e^{-\alpha_t} & \text{if } h_t(x_i) = y_i \\ e^{\alpha_t} & \text{if } h_t(x_i) \neq y_i \end{cases} \\ &= \frac{D_t(i) \exp(-\alpha_t y_i h_t(x_i))}{Z_t} \end{aligned}$$

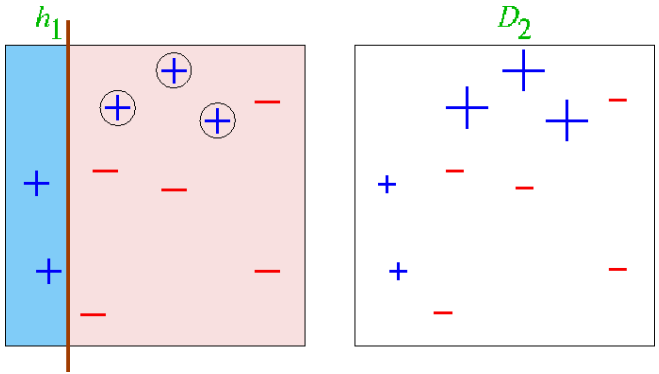
where Z_t is a normalization factor (chosen so that D_{t+1} will be a distribution).

Output the final hypothesis:

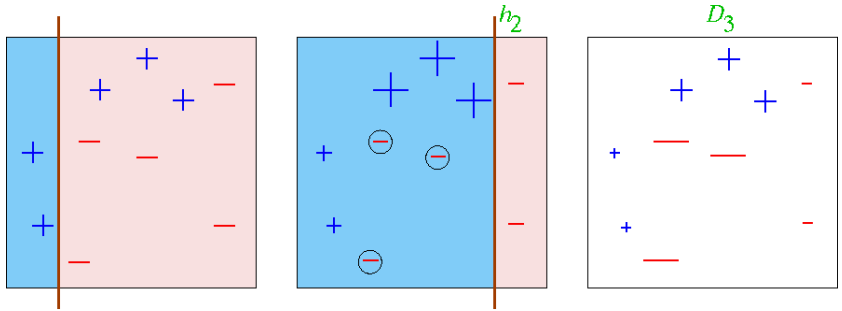
$$H(x) = \text{sign}\left(\sum_{t=1}^{T} \alpha_t h_t(x)\right).$$

Won the Gödel Prize in 2003.

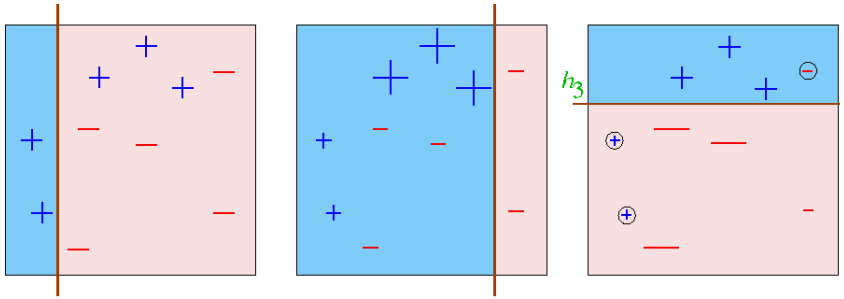
Example: First step



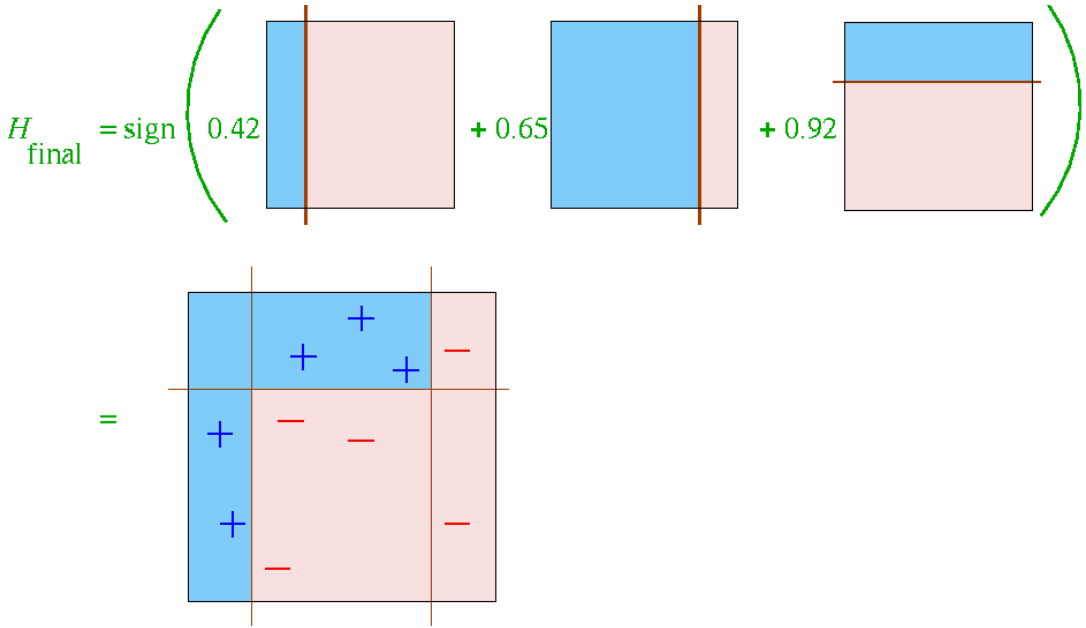
Example: Second step



Example: Third step



Example: Final hypothesis



Properties of AdaBoost

- Compared to other boosting algorithms, main insight is to automatically adapt the error rate at each iteration.

- Training error on the final hypothesis is at most:

$$\prod_t \left[2\sqrt{\epsilon_t(1-\epsilon_t)} \right] = \prod_t \sqrt{1-4\gamma_t^2} \leq \exp\left(-2 \sum_t \gamma_t^2 \right)$$

recall: γ_t = how much better than random is h_t

- AdaBoost gradually reduces the training error exponentially fast.

Why does boosting work?

Why does boosting work?

- Weak learners have high bias. By combining them, we get more expressive classifiers. Hence, boosting is a bias-reduction technique.

Why does boosting work?

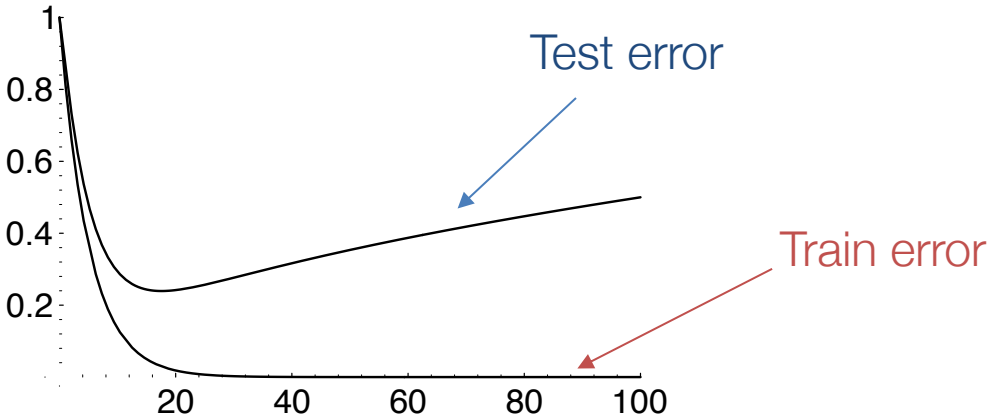
- Weak learners have high bias. By combining them, we get more expressive classifiers. Hence, boosting is a bias-reduction technique.

- Adaboost looks for a good approximation to the log-odds ratio, within the space of functions that can be captured by a linear combination of the base classifiers.

- What happens as we run boosting longer? Intuitively, we get more and more complex hypotheses. How would you expect bias and variance to evolve over time?

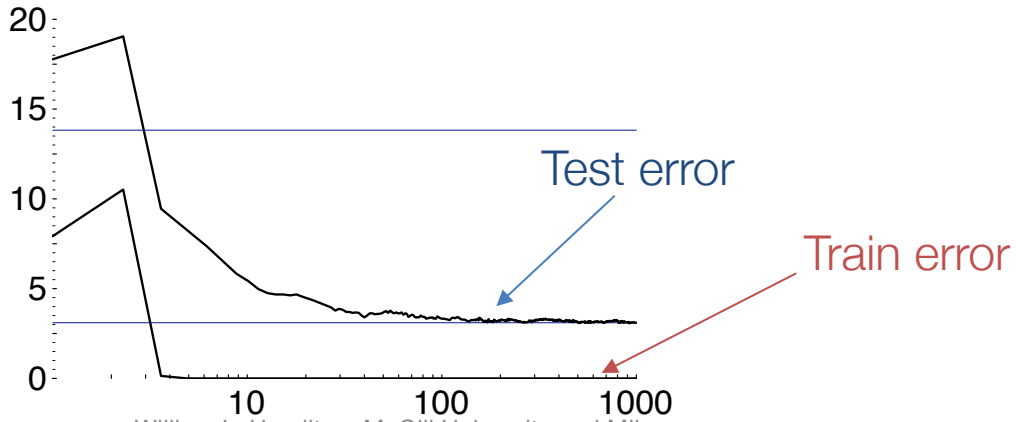
A naïve (but reasonable) analysis of error

- Expect the training error to continue to drop (until it reaches 0).
- Expect the test error to increase as we get more voters, and $\mathbf{h}_f$ becomes too complex.



Actual typical run of AdaBoost

- Test error does not increase even after 1000 runs! (more than 2 million decision nodes!)
- Test error continues to drop even after training error reaches 0!
- These are consistent results through many sets of experiments!
- Conjecture: Boosting does not overfit!



Bagging vs Boosting

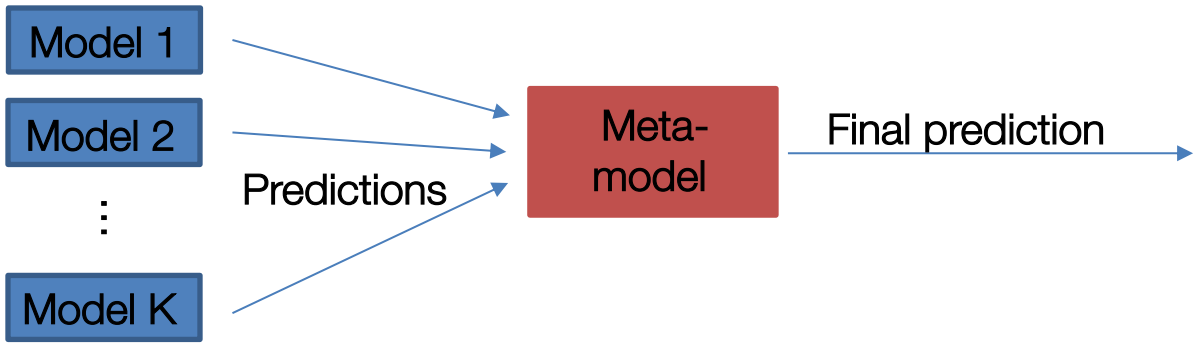
- Bagging is typically faster, but may get a smaller error reduction (not by much).
- Bagging works well with “reasonable” classifiers.
- Boosting works with very simple classifiers.
  - E.g., Boostexter - text classification using decision stumps based on single words.
- Boosting may have a problem if a lot of the data is mislabeled, because it will focus on those examples a lot, leading to overfitting.

Stacking

- Both bagging and boosting assume we have a single "base learning" algorithm.
- But what if we want to ensemble an arbitrary set of classifiers?
  - E.g., combine the output of a naïve Bayes and a nearest neighbor model?

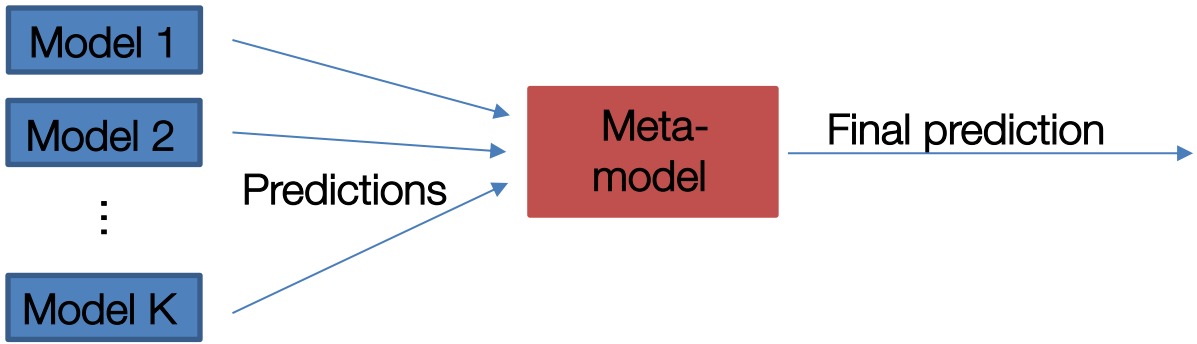
Stacking

- Both bagging and boosting assume we have a single "base learning" algorithm.
- But what if we want to ensemble an arbitrary set of classifiers?
  - E.g., combine the output of a naïve Bayes, and a nearest neighbor model?



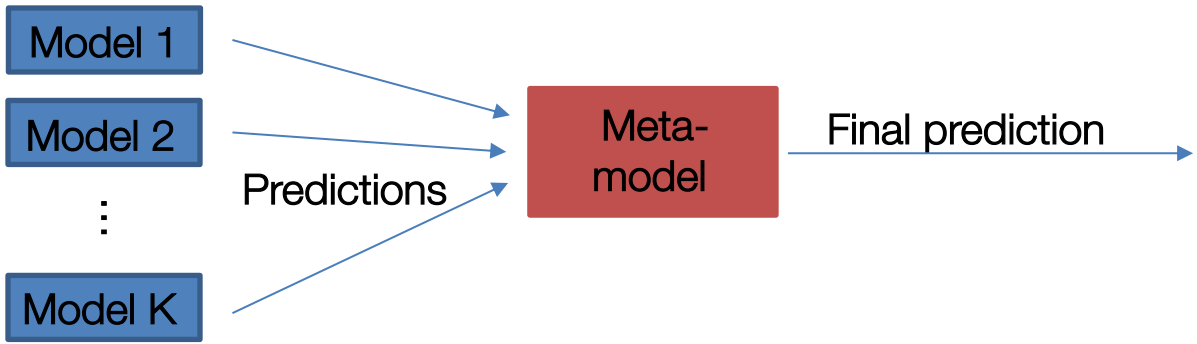
Stacking

- Train K distinct base models, h_k, $k=1...K$, on the training set $<x_i, y_i>$, $i=1...n$
- Make a new training set where the new features are the predictions of the base models: $<h_1(x_i), h_2(x_i), ..., h_K(x_i), y_i>$, $i=1...n$
  - (Can also add the original feature information, x_i, to the new training set)
- Train a meta-model m on this new training set.
  - (Possibly train multiple meta-models and repeat the process.)



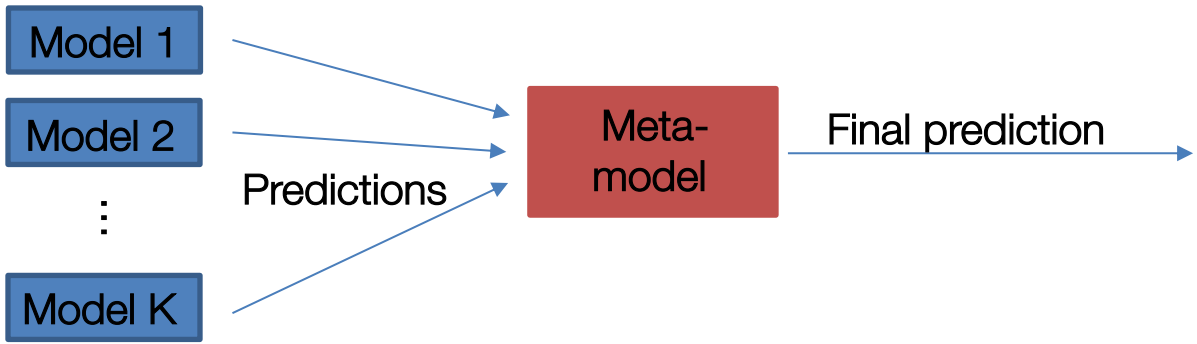
Meta-model

- What is the meta-model? Any supervised model will work!
- Common choices:
  - Averaging (for regression tasks)
  - Majority vote (for classification tasks)
  - Linear regression (for regression tasks)
  - Logistic regression (for classification tasks)



When does stacking work?

- Stacking works best when the base models have complimentary strengths and weaknesses (i.e., different inductive biases).
- For example: combining k-nearest neighbor models with different k-values, Naïve Bayes, and logistic regression. Each of these models has different underlying assumptions so (hopefully) they will be complimentary.



What you should know

- Ensemble methods combine several hypotheses into one prediction.
- They work better than the best individual hypothesis from the same class because they reduce bias or variance (or both).
- Bagging is mainly a variance-reduction technique, useful for complex hypotheses.
- Boosting focuses on harder examples, and gives a weighted vote to the hypotheses.
- Boosting works by reducing bias and increasing classification margin.
- Stacking is a generic approach to ensemble various models and performs very well in practice.