Ensemble

Big Data Lectures - Chapter 6

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Outline

- ▶ list of topics:
 - neural networks and deep learning
 - boosting
 - random forest
 - more ensemble methods



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Neural Networks and Deep Learning

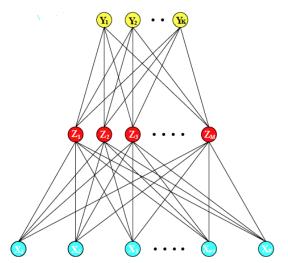


- neural networks:
 - the term has evolved to encompass a large class of models and learning methods, especially popular in the field of artificial intelligence, computer vision, and automatic speech recognition
 - we describe a widely used neural net, sometimes called the single hidden layer back-propagation network, or single layer perceptron
- examples:
 - a typical neural network used 1 to 10 million connections
 - ► Google Brain neural network used more than 1 billion connections developed a distributed computing infrastructure and spread the computation across 16,000 of our CPU cores



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key idea: sum of nonlinear functions of linear combinations of the inputs, typically represented by a network diagram





neural networks model:

$$Z_m = \sigma(\alpha_{0m} + \boldsymbol{\alpha}_m^{\mathsf{T}} \boldsymbol{X}), \quad m = 1, ..., M$$

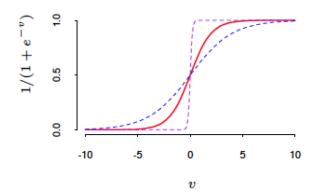
 $T_k = \beta_{0k} + \boldsymbol{\beta}_k^{\mathsf{T}} \boldsymbol{Z}, \quad k = 1, ..., K$
 $f_k(\boldsymbol{X}) = g_k(T), \quad k = 1, ..., K$

- **Y** = $(Y_1, ..., Y_K)$ are the K-dimensional output; e.g., for univariate response, K = 1; for K-class classification, kth unit models the probability of class k
- $ightharpoonup X = (X_1, \dots, X_p)$ are the p-dimensional input features
- ▶ $Z = (Z_1, ..., Z_M)$ are the derived features created from linear combinations of the inputs X
- ▶ $T = (T_1, ..., T_K)$ are the output features that are directly associated with the outputs Y through output functions $g_k(\cdot)$
- $g_k(T) = T$ for regression; $g_k(T) = e^{T_k} / \sum_{l=1}^K e^{T_l}$ for K-class classification



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- activation function:
 - usually $\sigma(v) = sigmoid = 1/(1 + e^{-v})$
 - $\sigma(v)$ = a step function: human brain models where each unit represents a neuron, and the connections represent synapses; the neurons fired when the total signal passed to that unit exceeded a certain threshold





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▶ loss function: residual sum of squares / deviance

$$L = \sum_{i=1}^{n} \sum_{k=1}^{K} (y_{ik} - f_k(x_i))^2, \qquad L = -\sum_{i=1}^{n} \sum_{k=1}^{K} y_{ik} \log f_k(x_i)$$

- model fitting: back propagation gradient descent
 - gradient descent update:

$$\beta_{km}^{(r+1)} = \beta_{km}^{(r)} - \gamma_r \sum_{i=1}^n \frac{\partial R_i}{\partial \beta_{km}} \qquad \alpha_{ml}^{(r+1)} = \alpha_{ml}^{(r)} - \gamma_r \sum_{i=1}^n \frac{\partial R_i}{\partial \alpha_{ml}}$$

where
$$R_{i} = \sum_{k=1}^{K} (y_{ik} - f_{k}(x_{i}))^{2}$$

• the derivatives: letting $z_{mi} = \sigma(\alpha_{0m} + \alpha_m^T x_i)$

$$\frac{\partial R_i}{\partial \beta_{km}} = -2(y_{ik} - f_k(x_i))g'_k(\beta_k^{\mathsf{T}} z_i)z_{mi} \equiv \delta_{ki} z_{mi}$$

$$\frac{\partial R_i}{\partial \alpha_{ml}} = -\sum_{k=1}^{K} 2(y_{ik} - f_k(x_i))g_k'(\beta_k^{\mathsf{T}} z_i)\beta_{km}\sigma'(\alpha_m^{\mathsf{T}} x_i)x_{il} \equiv s_{mi}x_{il}$$



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- model fitting: back propagation (continued)
 - lacktriangle δ_{ki} and s_{mi} are the "errors" from the current model at the output and hidden layer units
 - back propagation equations

$$s_{mi} = \sigma'(\alpha_m^\mathsf{T} x_i) \sum_{k=1}^K \beta_{km} \delta_{ki}$$

- two-pass updates:
 - forward pass: fix the current weights and compute the predicted values $\hat{f}_k(x_i)$
 - backward pass: compute the errors δ_{ki} , then back-propagate to compute the errors s_{mi}
 - update $\hat{\beta}_{km}$ and $\hat{\alpha}_{ml}$
- $ightharpoonup \gamma_r$ is the learning rate
- advantages: simple and local nature; each hidden unit passes and receives information only to and from units that share a connection can be implemented efficiently on a parallel architecture computer.

- practical issues:
 - starting values: usually starting values for weights are chosen to be random values near zero; hence the model starts out nearly linear, and becomes nonlinear as the weights increase
 - overfitting: early stopping; weight decay
 - scaling of the inputs: mean zero and standard deviation one
 - how many hidden units; how many hidden layers: guided by domain knowledge and experimentation
 - multiple minima: try with different starting values



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 - multiple minima: try with different starting values
- neural networks model is a projection pursuit type additive model:

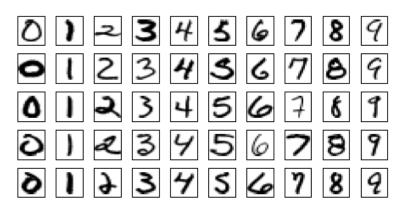
$$f(\boldsymbol{X}) = \beta_0 + \sum_{m=1}^{M} \beta_m \, \sigma(\alpha_{m0} + \boldsymbol{\alpha}_m^\mathsf{T} \boldsymbol{X})$$

view: neural networks are not a fully automatic tool, as they are sometimes advertised; as with all statistical models, subject matter knowledge should and often be used to improve their performancement.

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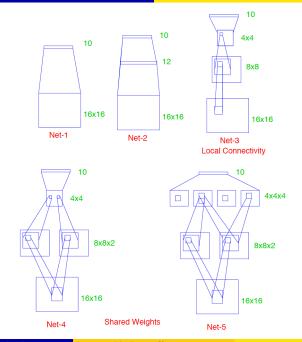
Example - handwritten digits

- 7IP code data:
 - ▶ input: 256 pixel values from 16 × 16 grayscale images; output: 0,1,...,9 10-class classification
 - ▶ a modest experimental subset: 320 training digits and 160 testing digits





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Example – handwritten digits

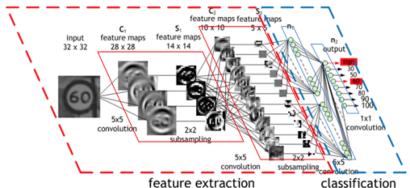
- neural networks used:
 - ▶ net-1: no hidden layer, equivalent to multinomial logistic regression
 - ▶ net-2: one hidden layer, 12 hidden units fully connected
 - net-3: two hidden layers locally connected
 - net-4: two hidden layers, locally connected with weight sharing
 - net-5: two hidden layers, locally connected, two levels of weight sharing (was the result of many person years of experimentation)
- results:

network	links	weights	accuracy
net 1	2570	2570	80.0%
net 2	3124	3214	87.0%
net 3	1226	1226	88.5%
net 4	2266	1131	94.0%
net 5	5194	1060	98.4%



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- deep learning is a class of machine learning algorithms that:
 - use a cascade of multiple layers of nonlinear processing units, and each successive layer uses the output from the previous layer as input





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convolution:

- a mathematical operation that describes a rule of how to mix two functions or pieces of information
- ▶ the feature map (the input data) + the convolution kernel ⇒ a transformed feature map
- convolution is often interpreted as a filter, where the kernel filters the feature map for information of a certain kind; e.g., one kernel might filter for edges and discard other information

Input image



Convolution Kernel

$$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$$

Feature map



1	1,	1,0	0,,1	0
0	1,0	1,	1,0	0
0	0,,1	1,0	1,	1
0	0	1	1	0
0	1	1	n	C

Image

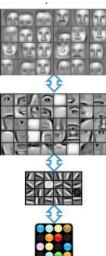


Convolved Feature



- hierarchical feature representation:
 - form a hierarchical representation of the data, where higher level features are derived from lower level features
 - image recognition: pixel → edge → motif → part → object
 - Speech: sample → spectral band → sound → phoneme → word
- ▶ feature engineering *vs* feature learning
 - feature engineering: extract useful features from the data for a specific learning task
 - feature learning: feature engineering automatically done by algorithms

 the learnt features are usually difficult to interpret





- challenges of a deep network:
 - computation hardware advancement, e.g., graphics processing unit (GPU)
 - vanishing gradients: the gradients became too small to provide a learning signal for very deep layers, thus making the deep architectures perform poorly when compared to shallow learning algorithms pre-trained one level at a time through unsupervised learning, then further fine-tuned through supervised back-propagation, alternative activation functions, alternative network structures . . .
- deep architectures:
 - ▶ feed-forward: multilayer neural networks, convolutional neural networks
 - ▶ feed-back: stacked sparse coding, deconvolutional nets
 - ▶ bi-drectional: deep Boltzmann machines, stacked auto-encoders



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- learning protocols:
 - purely supervised
 - initialize parameters randomly
 - train in supervised mode using back-propagation to compute gradients
 - used in most practical systems for speech and image recognition
 - unsupervised & layerwise + supervised classifier on top
 - train each layer unsupervised, one after the other
 - train a supervised classifier on top, keeping the other layers fixed
 - good when very few labeled samples are available
 - unsupervised & layerwise + global supervised fine-tuning
 - train each layer unsupervised, one after the other
 - add a classifier layer, and retrain the whole thing supervised
 - good when label set is poor



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Boosting



Boosting

- introduction:
 - boosting is one of the most powerful learning ideas introduced in the last twenty years (early this century)
 - it was originally designed for classification problems, while it can profitably be extended to regression as well
 - motivation: combines the outputs of many "weak" classifiers (e.g., classification trees) to produce a powerful "committee"
- history and literatures
 - ► AdaBoost: the most popular boosting algorithm by Freund and Schapire (1997)
 - ▶ Breiman (NIPS Workshop, 1996) referred to AdaBoost with trees as the "best off-the-shelf classifier in the world"
 - Friedman et al. (2000) offered a statistical view of the AdaBoost: a forward stagewise additive model with exponential loss
 - ► Friedman (2001) developed gradient boosting machine
 - debate between Mease and Wyner (2008) and Friedman et al. (20 review by Bühlmann and Hothorn (2007)

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AdaBoost

- consider a two-class classification problem:
 - ▶ $Y \in \{-1, 1\}$, the classifier G(x) has training error $\bar{\text{err}} = \frac{1}{n} \sum_{i=1}^{n} I(y_i \neq G(x_i))$
 - the expected error rate on future predictions is $E_{X,Y}I(Y \neq G(X))$
- ▶ the procedure:
 - sequentially apply the weak classification algorithm to repeatedly modified versions of the data
 - ▶ produces a sequence of weak classifiers $G_m(\mathbf{x}), m = 1, 2, ..., M$
 - ▶ the predictions from G_m 's are then combined through a weighted majority vote to produce the final prediction

$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(\mathbf{x})\right)$$

- ▶ the weights $\alpha_1, ..., \alpha_M$ are computed by the boosting algorithm:
 - they weigh the contribution of each G_m
 - give higher influence to more accurate classifiers in the sequence

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FINAL CLASSIFIER.

FINAL CLASSIFIER
$$G(x) = \operatorname{sign} \left[\sum_{m=1}^{M} \alpha_m G_m(x) \right]$$
Weighted Sample $G_3(x)$

Weighted Sample $G_2(x)$

Training Sample $G_1(x)$



AdaBoost

algorithm:

initialize: observation weights $w_i = 1/n, i = 1,...,n$ for m = 1,...,M do

fit a classifier $G_m(x)$ to the training data using weights w_i compute the weighted error

$$\operatorname{err}_m = \frac{\sum_{i=1}^n w_i I(y_i = G_m(\mathbf{x}_i))}{\sum_{i=1}^n w_i}$$

compute the **importance** of G_m as

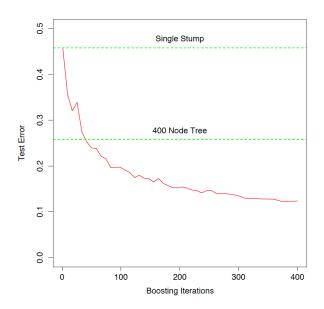
$$\alpha_m = \log(\frac{1 - \operatorname{err}_m}{\operatorname{err}_m})$$

update $w_i \leftarrow w_i \cdot \exp[\alpha_m \cdot I(y_i \neq G_m(\mathbf{x}_i))], i = 1, ..., n$ end for output $G(\mathbf{x}) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(\mathbf{x})\right)$



AdaBoost

- data modification in AdaBoost:
 - ▶ at each boosting step, apply weights $w_1, ..., w_n$ to the training observations $(x_i, y_i), i = 1, ..., n$
 - initially, all of the weights are set to $w_i = 1/n$
 - ▶ at step m = 2, 3, ..., M, those observations misclassified by $G_{m-1}(\mathbf{x})$ have weights increased; observations correctively classified by $G_{m-1}(\mathbf{x})$ have weights decreased
 - observations that are difficult to correctly classify receive ever increasing influence
 - each successive classifier is forced to concentrate on those training observations that are misclassified by previous classifiers
- ▶ an illustrative example:
 - ten features $X_1,...,X_{10} \sim N(0,1)$
 - two classes: $Y = 2 \cdot I(\sum_{i=1}^{10} X_i^2 > \chi_{10}^2(0.5)) 1$
 - raining size n = 2000, test size 10,000
 - weak classifier: stump (a two-terminal node classification tree)
 - ▶ misclassification error rate: stump 46%; 400-mode tree 26%; boosting 12.2%





Boosting as additive model

▶ boosting is an additive model:

$$G(\mathbf{x}) = \operatorname{sign}\left(\sum_{m=1}^{M} \alpha_m G_m(\mathbf{x})\right).$$

- fitting an additive expansion in a set of "basis" functions $G_m(x)$
- additive models: more generally, basis function expansions take the form

$$f(\mathbf{x}) = \sum_{m=1}^{M} \beta_m b(\mathbf{x}; \gamma_m)$$

- \triangleright β_m 's are expansion coefficients
- $b(x, \gamma_m)$ are simple functions of x, characterized by parameters γ_m



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Boosting as additive model

- model estimation via a loss function:
 - squared-error or likelihood-based loss functions
 - typically, the model is obtained by minimizing the loss function averaged over the training data

$$\min_{\beta_m, \gamma_{m_1}} \sum_{i=1}^n L\left(y_i, \sum_{m=1}^M \beta_m b(\mathbf{x}_i; \boldsymbol{\gamma}_m)\right)$$

 it is feasible to rapidly solve the subproblem of fitting just a single basis

$$\min_{\beta,\gamma} \sum_{i=1}^{n} L(y_i, \beta b(\mathbf{x}_i; \gamma))$$

- examples:
 - ightharpoonup CART uses step basis functions, γ parametrizes the split variables and points at the internal nodes, and the predictions at the terminal nodes

Boosting as additive model

- forward stagewise additive modeling:
 - approximate the function by sequentially adding new basis functions to the expansion without adjusting the parameters and coefficients of those that have been added.
 - ▶ at iteration m, one solves for the optimal basis function $b(x, \gamma_m)$ and corresponding coefficient β_m to add to the current expansion $f_{m-1}(x)$
- algorithm:

initialize
$$f_0(\mathbf{x}) = 0$$

for $m = 1, ..., M$ **do**
compute

$$(\beta_m, \gamma_m) = \arg\min_{\beta, \gamma} \sum_{i=1}^n L(y_i, f_{m-1}(\mathbf{x}_i) + \beta b(\mathbf{x}_i; \gamma))$$

set
$$f_m(x) = f_{m-1}(x) + \beta_m b(x; \gamma_m)$$

end for



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AdaBoost – a statistical view

- what is AdaBoost in a statistical view:
 - AdaBoost builds an additive logistic regression model

$$f(\mathbf{x}) = \log \frac{\Pr(Y = 1|\mathbf{x})}{\Pr(Y = -1|\mathbf{x})} = \sum_{m=1}^{M} \beta_m G_m(\mathbf{x})$$

- model fitting: forward stagewise additive modeling
- loss function: the exponential loss function

$$L(y, f(\mathbf{x})) = \exp[-yf(\mathbf{x})]$$

- ▶ the basis functions are individual classifiers $G_m(\mathbf{x}) \in \{-1, 1\}$.
- remarks:
 - the success of boosting is not that mysterious
 - why equivalent; how connects to a more familiar stat model; why exponential loss function



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AdaBoost – a statistical view

- compared to slide-25:
 - one needs to solve (β_m, G_m) to minimize

$$\sum_{i=1}^{n} \exp[-y_{i}(f_{m-1}(\mathbf{x}_{i}) + \beta G(\mathbf{x}_{i}))] = \sum_{i=1}^{n} w_{i}^{(m)} \exp[-\beta y_{i} G(\mathbf{x}_{i}))]$$

where $w_i^{(m)} = \exp[-y_i f_{m-1}(x_i)]$

- $w_i^{(m)}$ depends only on $f_{m-1}(x_i)$, not on β or G(x); weights
- the solution is updated as $f_m(\mathbf{x}) = f_{(m-1)}(\mathbf{x}) + \beta_m G_m(\mathbf{x})$:

$$G_m = \arg\min_{G} \sum_{i=1}^{m} w_i^{(m)} I(y_i \neq G(\mathbf{x}_i))$$

$$\beta_m = \frac{1}{2} \log \frac{1 - \operatorname{err}_m}{\operatorname{err}_m} = \frac{1}{2} \alpha_m$$

the weights for the next iteration are:

$$w_i^{(m+1)} = w_i^{(m)} \exp(-\beta_m y_i G_m(\mathbf{x}))$$

=
$$w_i^{(m)} \exp(\alpha_m I(y_i \neq G(\mathbf{x}_i))) \exp(-\beta_m)$$



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AdaBoost – a statistical view

what AdaBoost actually estimates:

$$f^*(\mathbf{x}) = \arg\min_{f} E_{Y|\mathbf{x}}[e^{-Yf(\mathbf{x})}] = \frac{1}{2} \log \frac{\Pr(Y=1|\mathbf{x})}{\Pr(Y=-1|\mathbf{x})}$$

- equivalently, $Pr(Y = 1 | x) = [1 + exp{-2f^*(x)}]^{-1}$
- ▶ the additive expansion produced by AdaBoost is estimating one half of the log-odds of $\Pr(Y = 1 | \mathbf{x})$
- another loss criterion with the same population minimizer:
 - the binomial negative log-likelihood (deviance / cross-entropy)
 - ▶ let $Y' = (Y+1)/2 \in \{0,1\}$, then the binomial negative log-likelihood loss function is

$$-I(Y, p(x)) = -[Y' \log p(x) + (1 - Y') \log(1 - p(x))]$$

= \log (1 + \exp(-2Yf(x)))

where
$$p(x) = [1 + e^{-2f(x)}]^{-1}$$

• the population minimizers of the deviance $E_{Y|x}[-l(Y, f(x))]$ and $E_{Y|x}[e^{-Yf(x)}]$ are the same.



Gradient boosting machine

- functional optimization view:
 - boosting as an optimization algorithm in functional space
 - ▶ this interpretation opens the door to understand what boosting does and brings boosting from classification to regression, survival ...
- gradient boosting machine: functional gradient descent

initialize $f_0(\mathbf{x}) = 0$ or an offset value

for $m = 1, \ldots, M$ do

compute the negative gradient and evaluate at $f_{m-1}(\mathbf{x}_i)$

$$g_{mi} = \left[-\frac{\partial L(y, f(\mathbf{x}))}{\partial f(\mathbf{x})} \right]_{f(\mathbf{x}) = f_{m-1}(\mathbf{x}_i)}$$

fit g_{mi} to x_i with a base learner: $\hat{g}_m(x, \gamma_m) : x_i \to g_{mi}$ line search:

$$\rho_{m} = \arg\min_{\rho} L(y, f_{m-1}(\mathbf{x}) + \rho \hat{\mathbf{g}}_{m}(\mathbf{x}, \boldsymbol{\gamma}_{m}))$$

update
$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \nu \rho_m \hat{\mathbf{g}}_m(\mathbf{x}, \boldsymbol{\gamma}_m)$$
 end for



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Gradient boosting machine

gradient for some common loss functions:

algorithm	loss function	negative gradient
AdaBoost	$\exp[-yf(x)]$	$y \exp[-yf(x)]$
LogitBoost	$\log\{1+\exp[-2yf(\boldsymbol{x})]\}$	$2y/\{1+\exp[2yf(\boldsymbol{x})]\}$
L_2 Boost	$\frac{1}{2}[y-f(x)]^2$	$y - f(\boldsymbol{x})$
LADBoost	y-f(x)	sign(y - f(x))

- base learner:
 - **component-wise** linear model: regression of g_{mi} on x_{ij} for j = 1, ..., p
 - component-wise smoothing splines
 - trees
- regularization:
 - early stopping: control the number of boosting iterations
 - shrinkage: a small shrinkage coefficient $0 < \nu < 1$
- ▶ theoretical investigation: Bühlmann and Yu (2003, JASA)



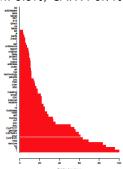
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Gradient boosting machine

interpretation: predictor relative importance

$$\left\{ E\left[\frac{\partial \hat{f}(\boldsymbol{X})}{\partial X_j}\right]^2 \operatorname{var}(X_j) \right\}^{1/2} \quad j = 1, \dots, p$$

- spam email data revisit:
 - boosting: 4.5%, GAM: 5.5%, CART: 8.7%





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Random Forests



Random forests

bagging:

- ► an additive model / committee method for reducing the variance of an estimated prediction function
- simply fit the same regression tree many times to bootstrap sampled versions of the training data, and average the result
- ▶ an average of B i.i.d. random variables, each with variance σ^2 , has variance $\frac{1}{B}\sigma^2$
- ▶ an average of B i.d. random variables, with positive pairwise correlation ρ , has variance $\rho \sigma^2 + \frac{1-\rho}{B} \sigma^2$

boosting:

- ▶ the committee of weak learners evolves over time
- the members cast a weighted vote

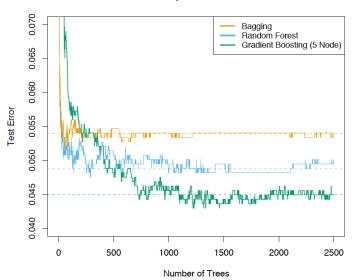
► random forest:

- ▶ a substantial modification of bagging that builds a large collection of de-correlated trees, and then averages them
- bagging is often dominated by boosting, whereas random forests enjoy
 a similar performance as boosting, and are simpler to train and terrer

Random forests

- algorithm:
 - for *b* = 1 to *B*:
 - draw a bootstrap sample of size n from the training data
 - grow a tree T_b to the bootstrapped data, by recursively repeating for each terminal node of the tree
 - select m variables at random from the p variables (de-correlation)
 - pick the best variable/split-point among them
 - split the node into two daughter nodes
 - output the ensemble of trees $\{T_b\}_1^B$
 - regression: $\hat{f}_B(\mathbf{x}) = \frac{1}{B} \sum_{b=1}^{B} T_b(\mathbf{x})$
 - classification: $\hat{C}_B(\mathbf{x}) = \text{majority vote } \{\hat{C}_b(T_b(\mathbf{x}))\}_1^B$
- remarks:
 - correlation reduction is achieved in the tree-growing process through random selection of the input variables
 - not all estimators can be improved by shaking up the data like this; it seems that highly nonlinear estimators, such as trees, benefit the increase.

Spam Data





Ensemble Methods



Ensemble methods

- introduction:
 - build a prediction model by combining (the strengths of) a collection of base models
 - two tasks: developing a number of base learners from the training data + combining them to form the composite predictor
- learning the ensemble:
 - lasso-based approach:

$$\min_{\alpha} \sum_{i=1}^{n} L[y_i, \alpha_0 + \sum_{m=1}^{M} \alpha_m T_m(\mathbf{x}_i)] + \lambda \sum_{m=1}^{M} |\alpha_m|$$

super learner



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Additional readings

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