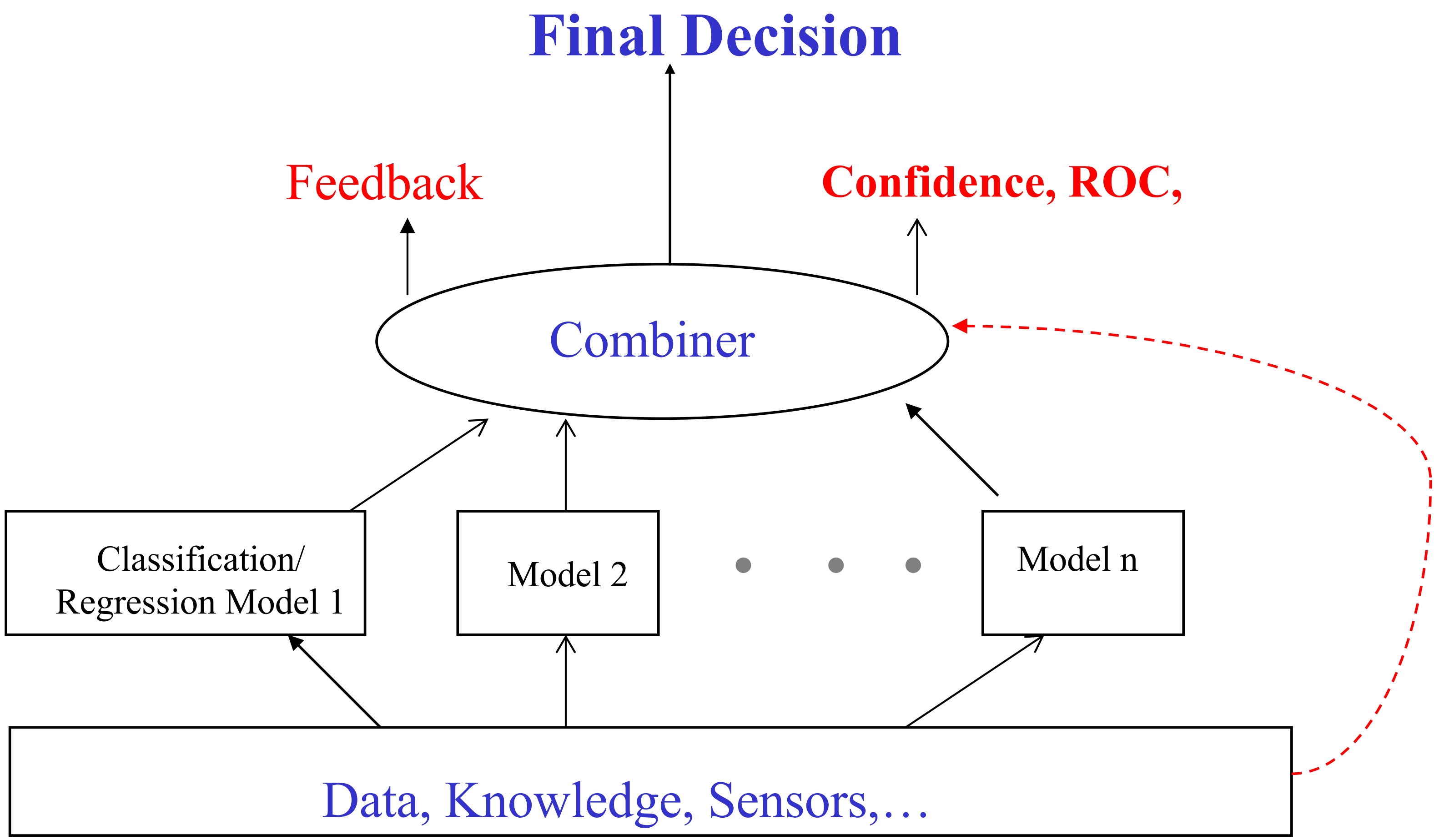
Ensembles and Multi-Learner Systems

- Goal
  - use multiple "learners" to solve (parts of) the same problem
    - Regression/ Function approximation
    - classification

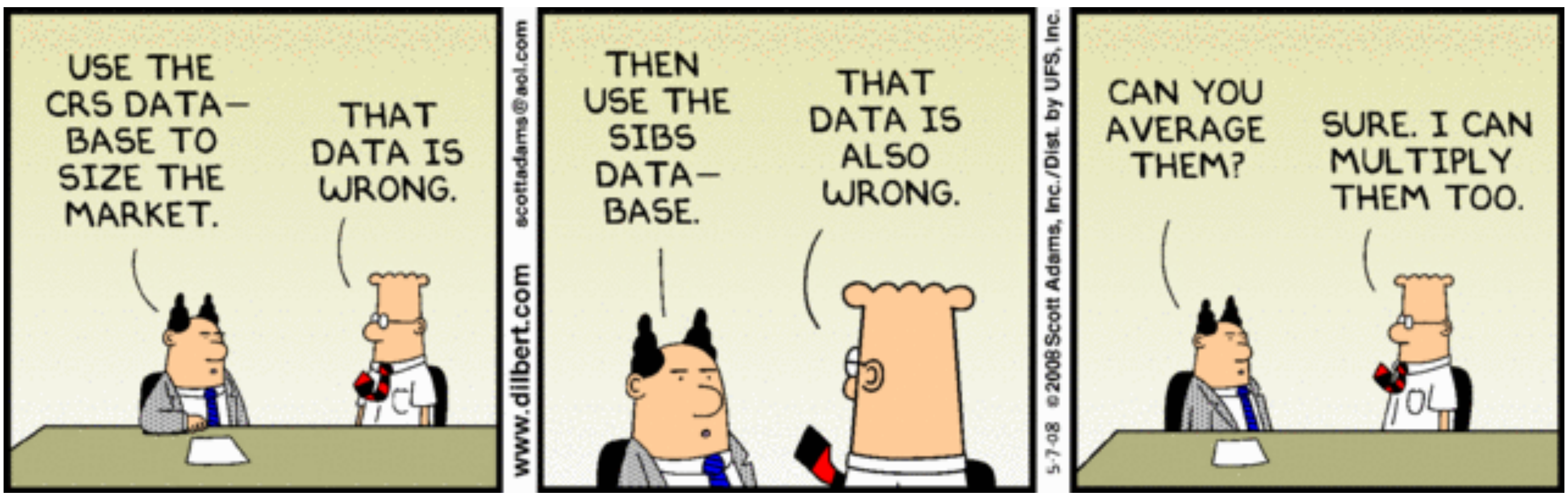
- Competing learners: ENSEMBLES
  - Multiple looks at same problem
- Cooperative learners: Mixture of experts and modular networks
  - Divide and conquer

Generic Multi-learner System



RoadMap

- Motivation
- Design Issues
- Lessons Learned



Motivation: Ensembles

- Different learners have different "inductive bias"
  - generalize differently from same training set
- Different properties
  - local vs. global
  - computation time / memory
  - susceptibility to outliers
- In designing/choosing one learner, several get created anyway!

- Hopes: better accuracy and better reliability

Very Early History

- Combining Votes/Ranks: Roots in French revolution!
  - Borda Counts: Jean-Claude de Borda, 1781
  - Condorcet's rule, 1785
    - Given rank orders, Select "person" who defeats all others in 1-1 contests

→ No notion of "true class", just the rankings

- Combining Estimators: Linear opinion pool (Laplace)

Hybrid Models in the 70’s and 80’s

Theory: *“No single model exists for all pattern recognition problems and no single technique is applicable to all problems. Rather what we have is a bag of tools and a bag of problems”* Kanal, 1974

Practice: multimodal inputs; multiple representations,…

- Syntactic + structural + statistical approaches to pattern recognition (PR) (Bunke 86)
- multistage models:
  - progressively identify/reject subset of classes
  - Cascade solutions, e.g. invoke KNN if linear classifier is ambiguous
- Combining multiple output types: 0/1; [0,1],…

→ Designs were typically specific to application

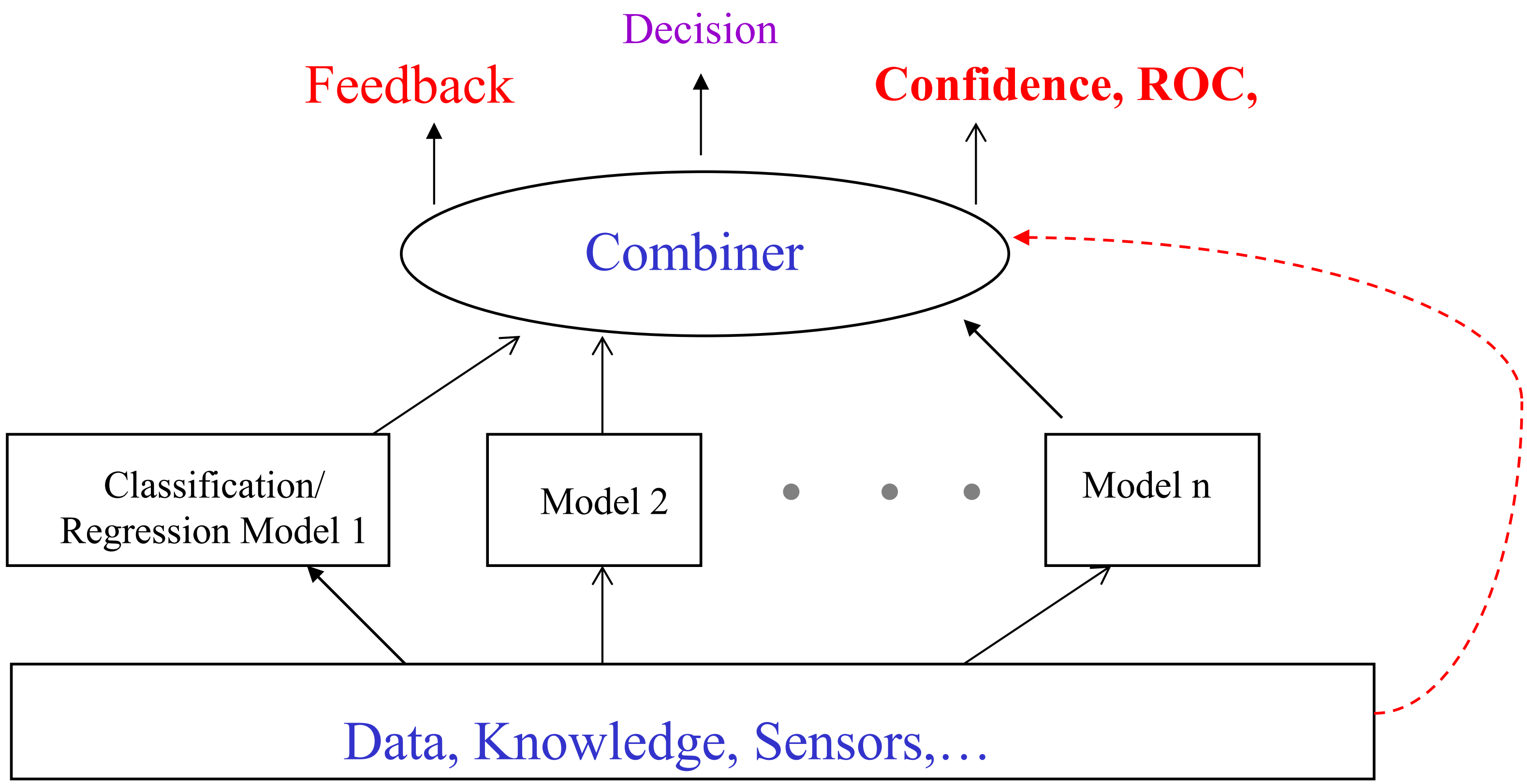
Combining Multiple Models in Other Areas

PR/Vision:	Data /sensor/decision fusion
AI:	evidence combination (Barnett 81)
Econometrics:	combining estimators (Granger 89)
Engineering:	Non-linear control
Statistics:	model-mix methods, Bayesian Model Averaging,..
Software:	diversity

….

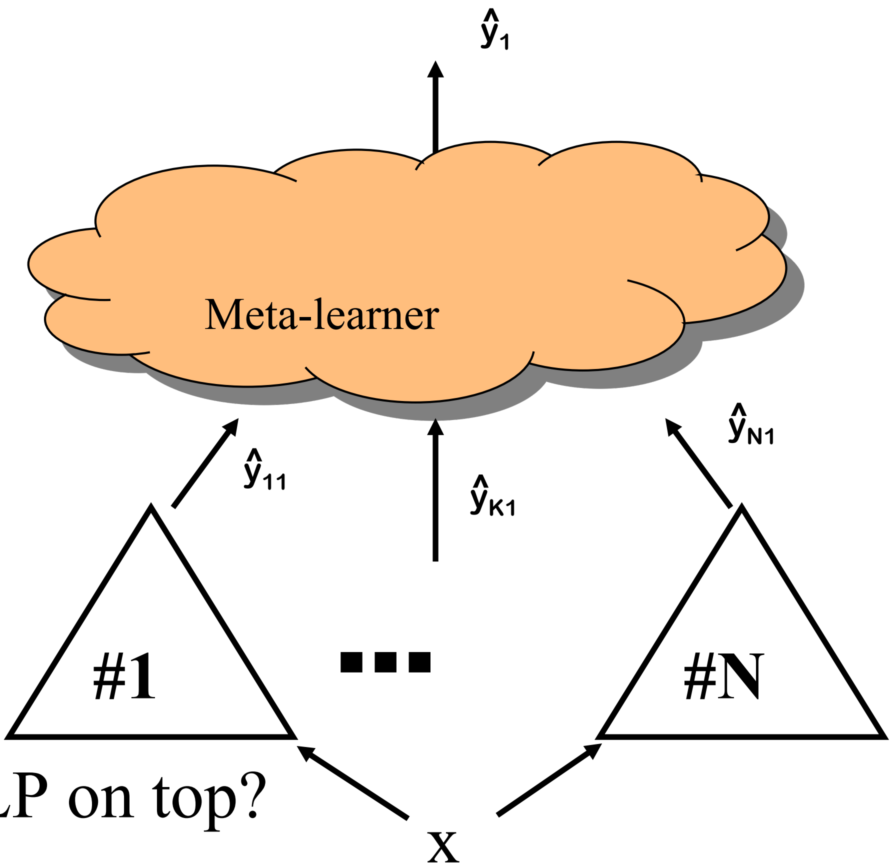
Common Issues

- Designing meta-learner or combiner
- Selecting the experts / learners / classifiers
- Determining training sets (same? automatic decomposition?)
- Estimating the gains, reliability



Output Combining for Function Approximation

- Meta-learners (trained)



- 1) Put a linear regressor or MLP on top?
- 2) Stacked Generalization (Wolpert 92)
  - train second layer model on leave-one-out samples

Problems?

Output Combining for Function Approximation
(cont.)

- 3) Weighted average (Hashem 93)

$$y_{av}(x) = \Sigma\, w_i y_i(x)\ ;$$
$$w_i \geq 0;\ \ \Sigma\, w_i = 1$$

  - Weights independent of x
  - Expression for Optimal weights involves inverse of C, the covariance matrix of the "mismatches"
    - Problem: entries of C are estimated, and rows are correlated
      - inversion →collinearity problems

- 4) More Practical: weight each model inversely proportional to its (estimated) MSE

Gains from the Averaging Combiner

- **Analysis of Ensemble based on Simple Averaging, i.e.**
- MSE of the "averaging" ensemble =
average value of MSE over models in the ensemble – average value of ambiguity of the individual models.

- Ambiguity= variance among the responses of different models for the same "x".

- So, need **good but diverse models**
    - rather overtrain than undertrain !!

Gains from the Averaging Combiner

- **Analysis of Ensemble based on Simple Averaging, i.e.**
- Define ambiguity for *i* th model, whose output is $y_i\ (x_j)$ for the j^{th} training point, as the average squared mismatch between its answer and the ensemble answer
- Ambiguity of *i* th model = $E_X\ [(y_i\ (x) - y^{ave}(x))^2]$

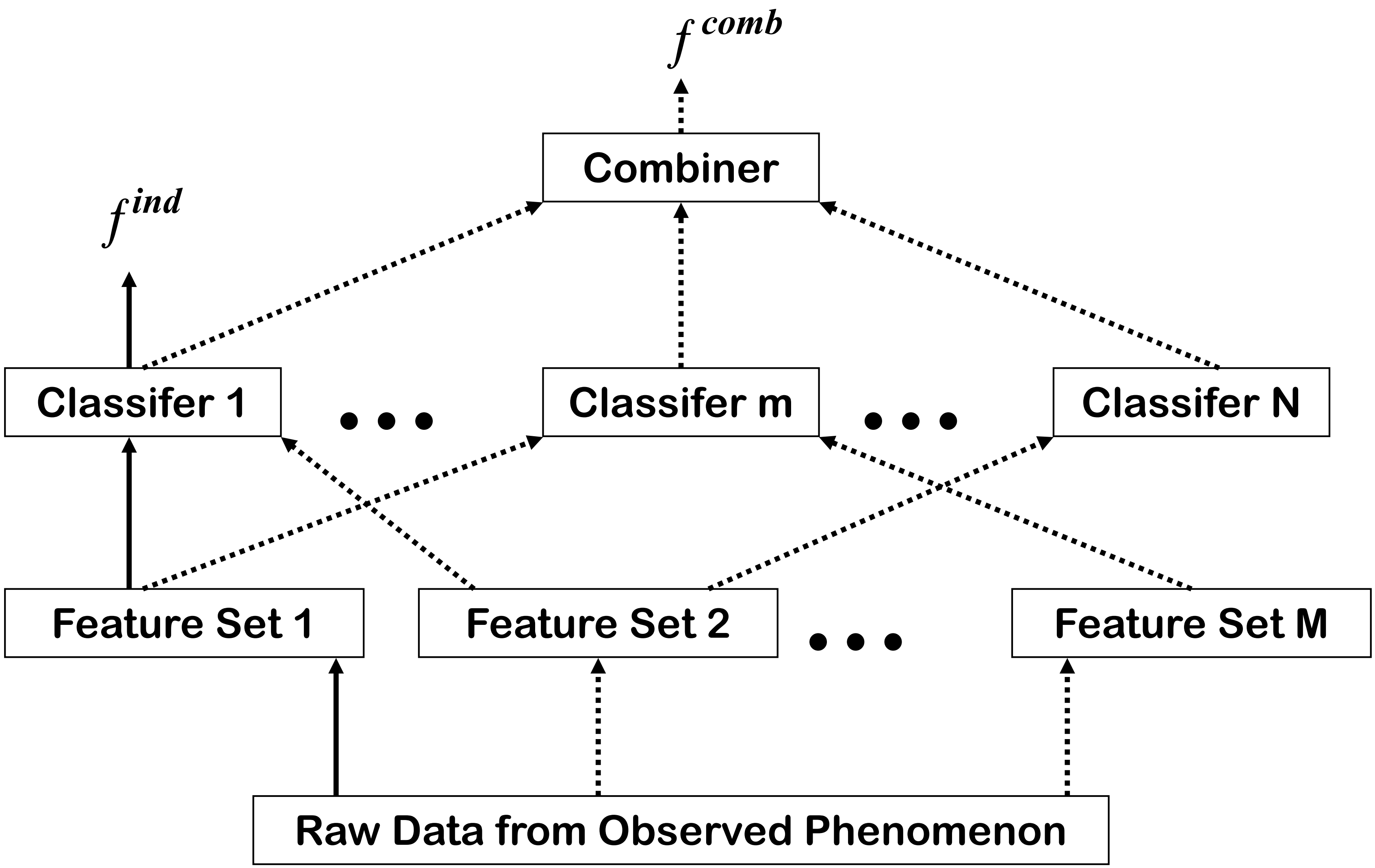
where $y^{ave}\ (x)$ is the ensemble answer (simple average)

- Can show MSE of the "averaging" ensemble = average value of MSE over models in the ensemble – average value of ambiguity of the individual models.

So, need **good but diverse models**

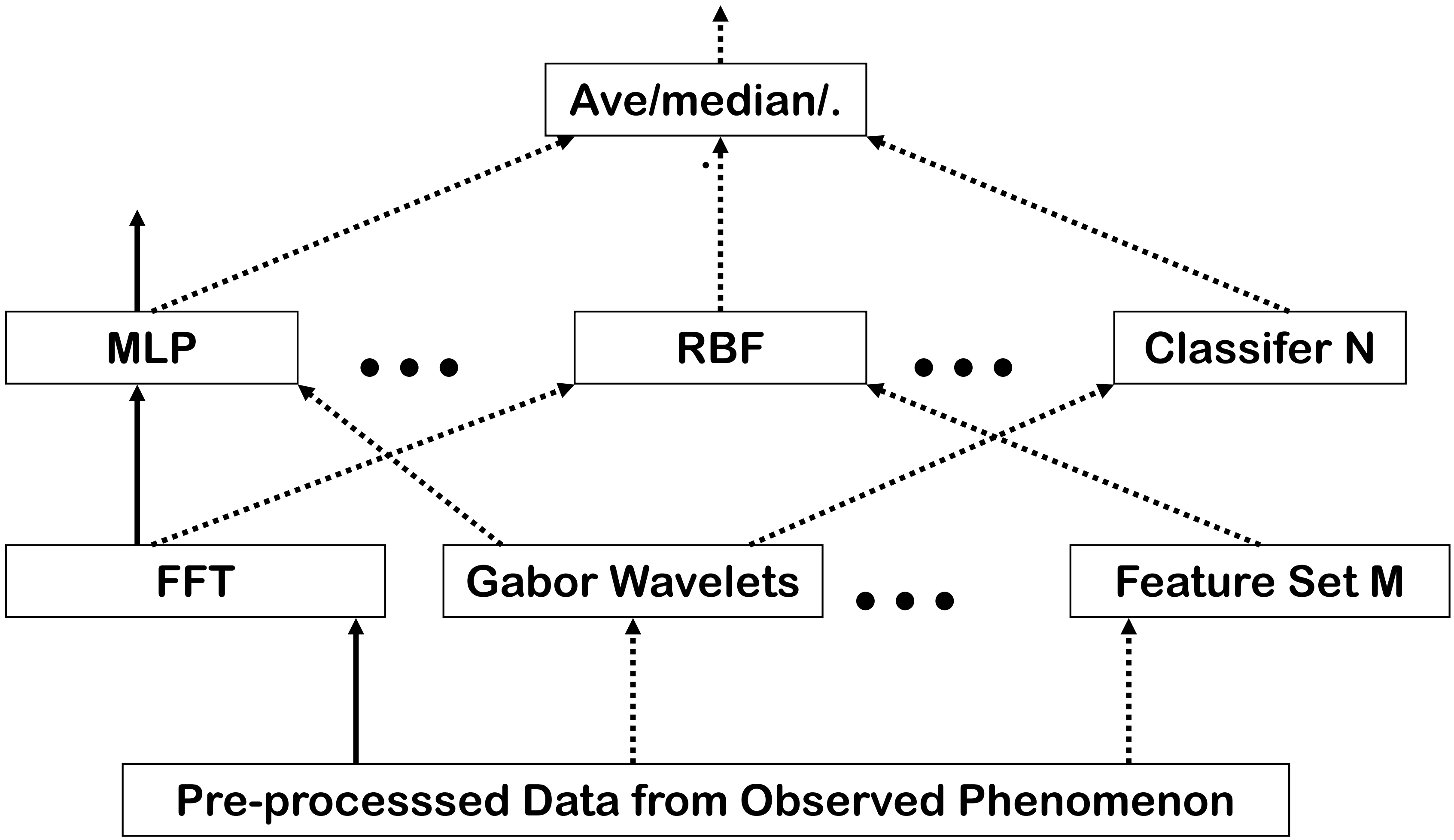
  - rather overtrain than undertrain !!

Multi-Classifier Systems (MCS)



DARPA Sonar Transients Classification Program (1989-)

J. Ghosh, S. Beck and L. Deuser, *IEEE Jl. of Ocean Engineering*, Vol 17, No. 4, October 1992, pp. 351-363.



MCS: Combining the Outputs

- Hard decisions? – majority vote (classic)
- Rank order available? – Borda counts, etc.
- Soft decisions? (e.g Posterior probability estimates) – treat as function approximation
- More complex methods: The Multisensor Fusion Framework (Dasarathy 94)
  - Communication costs; ROC effects considered
  - Typically solution is of form: coupled "weighted average of decisions compared to threshhold"

Output Combining of Soft Decisions

- Pick max. of (product; average; median; entropy weighting…)

- Best way?
  - Theory: (Kittler, Hatef & Duin, 96)
    - exact posteriors + independent assumptions => optimal solution is (weighted) product (Bayesian)
    - but product is much more susceptible to errors than average, median
  - Empirical: Average, median slightly better
  - Outliers? Order statistics combining
- How much can be gained?
  - Look at effect on decision boundaries (Tumer and Ghosh, 96)
    - gains "proportional" to lack of correlation among the errors in estimating the true posterior probabilities

Selecting the Inputs

- Bagging (Breiman, 92)
  - Gains where sensitivity is high
- Boosting (Schapire, 90)
  - Spl. Case of Adaptive Reweighting and Combining (ARC) methods
  - ***Read Ch 10 of HTF** for
    - Boosting and connections with Addition logistic regression
    - Gradient Boosted Decision Trees (GBDT)

Bagging (Bootstrap Aggregating)

- Variance reduction technique
- Method:
  - create bootstrap (sampling with replacement) replicates of dataset
  - fit a model to each replicate
  - combine predictions by averaging or voting
- Properties
  - stabilizes unstable models
    - **Decision trees**, neural nets
    - Prefer deeper trees (why??)
  - easily parallelizable; implementable
- Ref: www.stat.berkeley.edu/users/breiman/

Bagged Trees example from HTF Sec 8.7

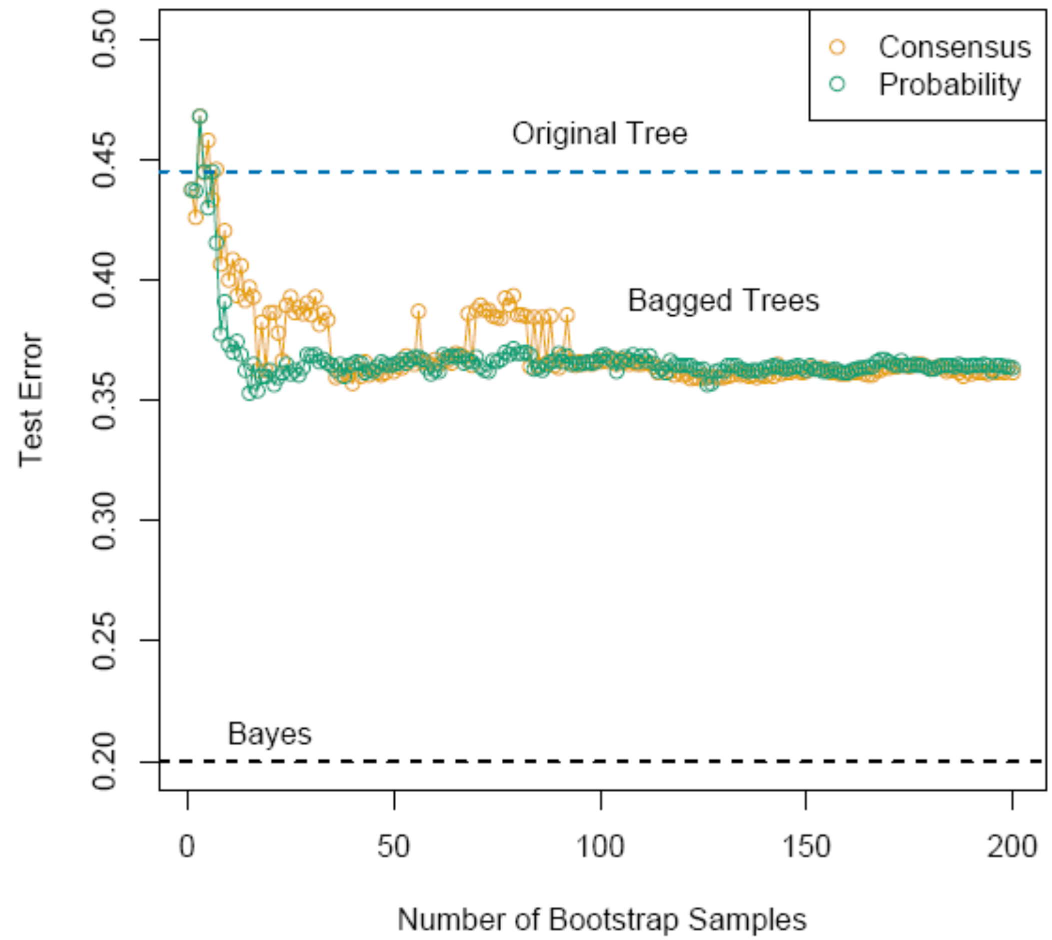
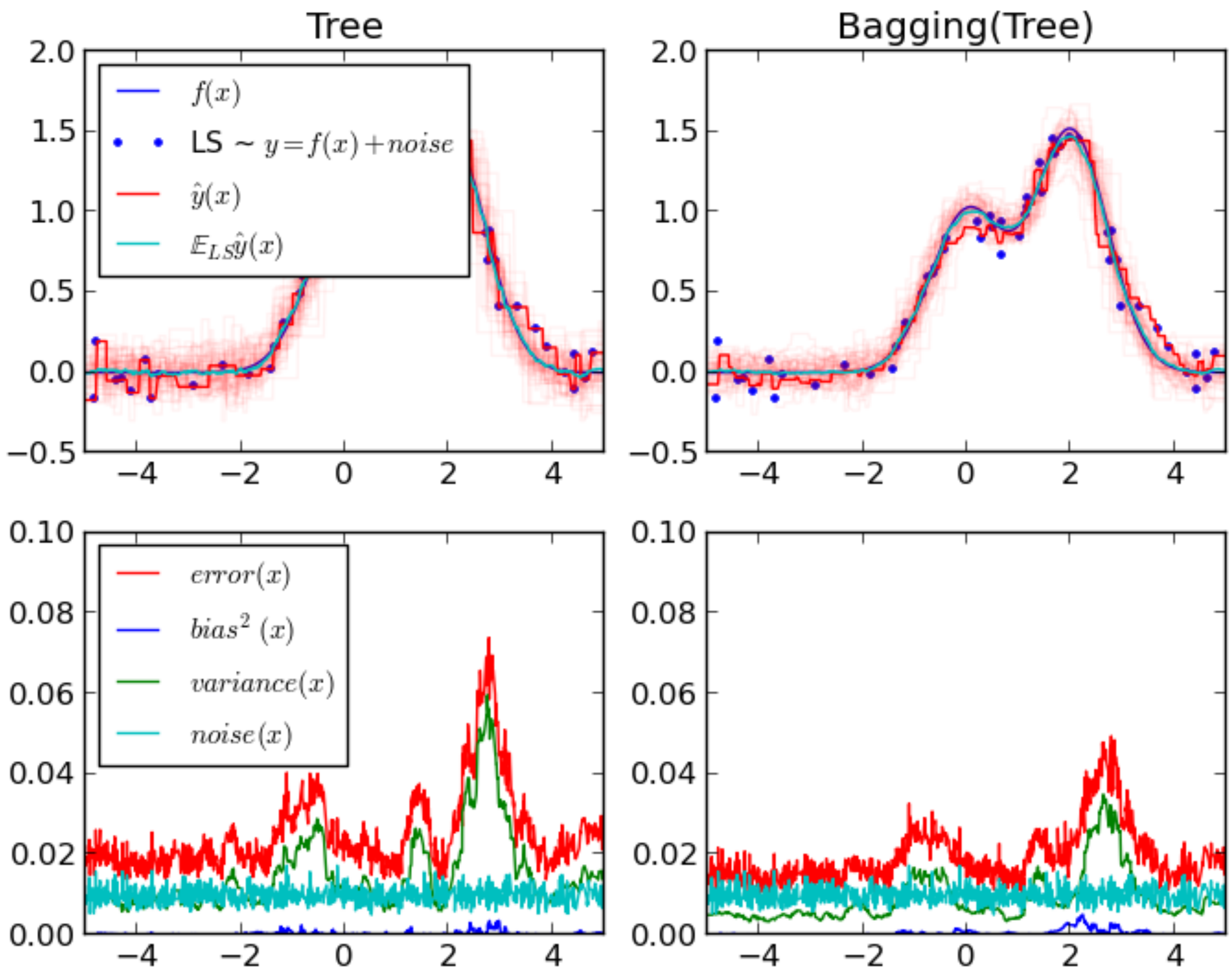


FIGURE 8.10. *Error curves for the bagging example of Figure 8.9. Shown is the test error of the original tree and bagged trees as a function of the number of bootstrap samples. The orange points correspond to the consensus vote, while the green points average the probabilities.*

Bagging Reduces Variance

http://scikit-learn.org/stable/auto_examples/ensemble/plot_bias_variance.html



Random Forests

- Bagging decision trees with additional randomization
  - generate bootstrap samples.
  - build one tree per bootstrap sample
  - increase diversity via additional randomization: randomly pick a subset of features of size $m << d$ to split at each node
    - Goal: Decrease correlation among trees without affecting bias much
    - Should determine *m* using out of bag (OOB) samples.
  - take equally weighted average of the results from each tree
- **Theory**: Variance of average of B (identically distributed, but not independent) variables = $\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$

Where ρ = pair-wise correlation and σ^2 is variance of each variable.

Random Forests

- R: randomForest
- Reduce correlation among bagged trees
  - Consider only subset of variables at each split

Algorithm 15.1 *Random Forest for Regression or Classification.*

1. For $b = 1$ to B:
   (a) Draw a bootstrap sample $\mathbf{Z}^*$ of size N from the training data.
   (b) Grow a random-forest tree T_b to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size n_{min} is reached.
      i. Select m variables at random from the p variables.
      ii. Pick the best variable/split-point among the m.
      iii. Split the node into two daughter nodes.
2. Output the ensemble of trees $\{T_b\}_1^B$.

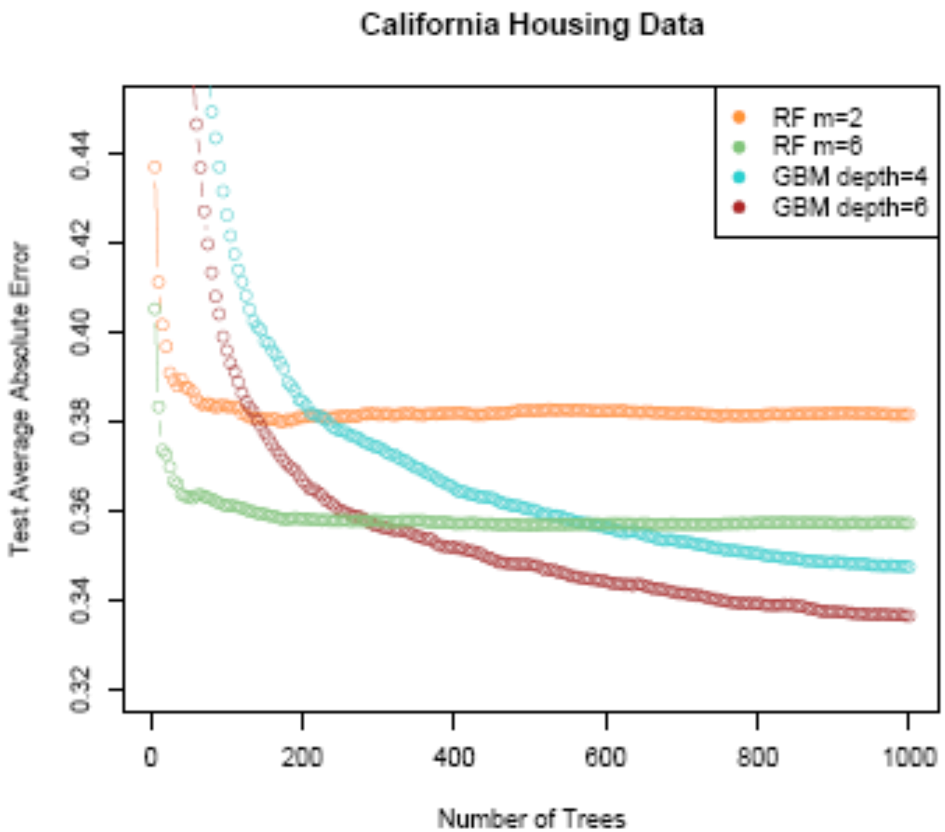
To make a prediction at a new point x:

Regression: $\hat{f}_{\text{rf}}^B(x) = \frac{1}{B}\sum_{b=1}^{B} T_b(x)$.

Classification: Let $\hat{C}_b(x)$ be the class prediction of the bth random-forest tree. Then $\hat{C}_{\text{rf}}^B(x) = \textit{majority vote}\ \{\hat{C}_b(x)\}_1^B$.

Performance

- Easy to train/tune
  - And can get variable importance like GBDT
- Typically better than bagging, often comparable to boosting, not as good as GBDT



Boosting

- Goal: improving classification, esp. with weak models
- Method:
  - sequentially fit models
  - later models see more of the samples mispredicted by earlier ones (input reweighting)
  - combine using weighted average (later models get more weight)
- Properties
  - reduces both bias and variance
  - slow to overfit
  - works well with "stumps", naïve Bayes,…
- Several Variations
- Danger: Sensitive to outliers

AdaBoost Algorithm

- **Note:** both outputs y_i and hypothesis (classifier) h_i are **+/- 1**

Input: Training set $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)$

Algorithm: Initialize $D_1(i) = 1/m$

For $t = 1, \ldots, T$

Weighted error

- Train a weak learner using distribution D_t
- Get weak hypothesis h_t with error $\epsilon_t = \Pr_{\mathbf{x} \sim D_t}[h_t(\mathbf{x}) \neq y]$
- Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\epsilon_t}{\epsilon_t}\right)$
- Update

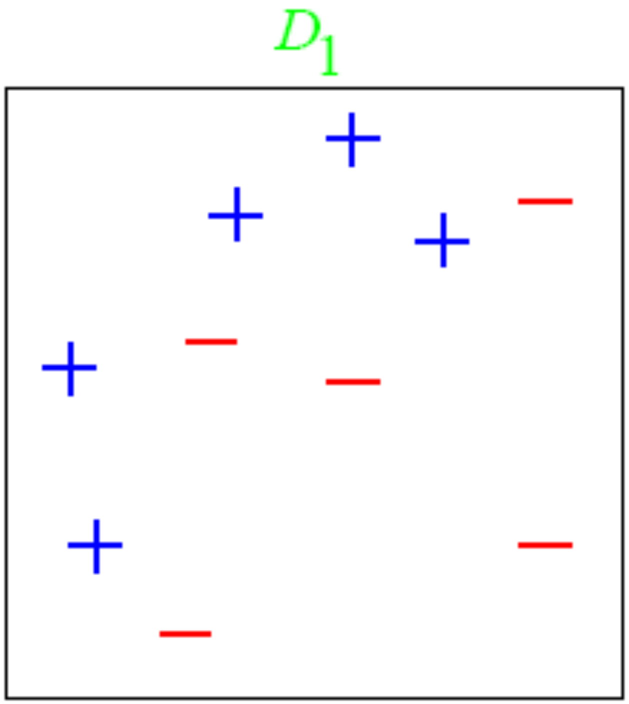
$$D_{t+1}(i) = \frac{D_t(i) \exp(-\alpha_t y_i h_t(\mathbf{x}_i))}{Z_t}$$

where Z_t is the normalization factor

Output: $h(\mathbf{x}) = \text{sign}(\sum_{t=1}^{T} \alpha_t h_t(\mathbf{x}))$

Toy Example from Schapire's NIPS 2007 tute

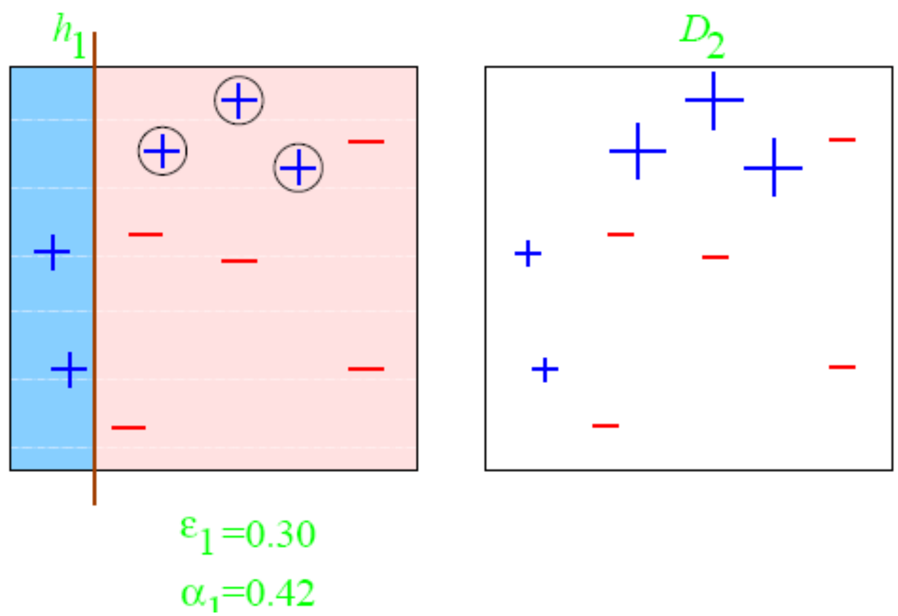
- Weak classifier: single horizontal or vertical half-plane



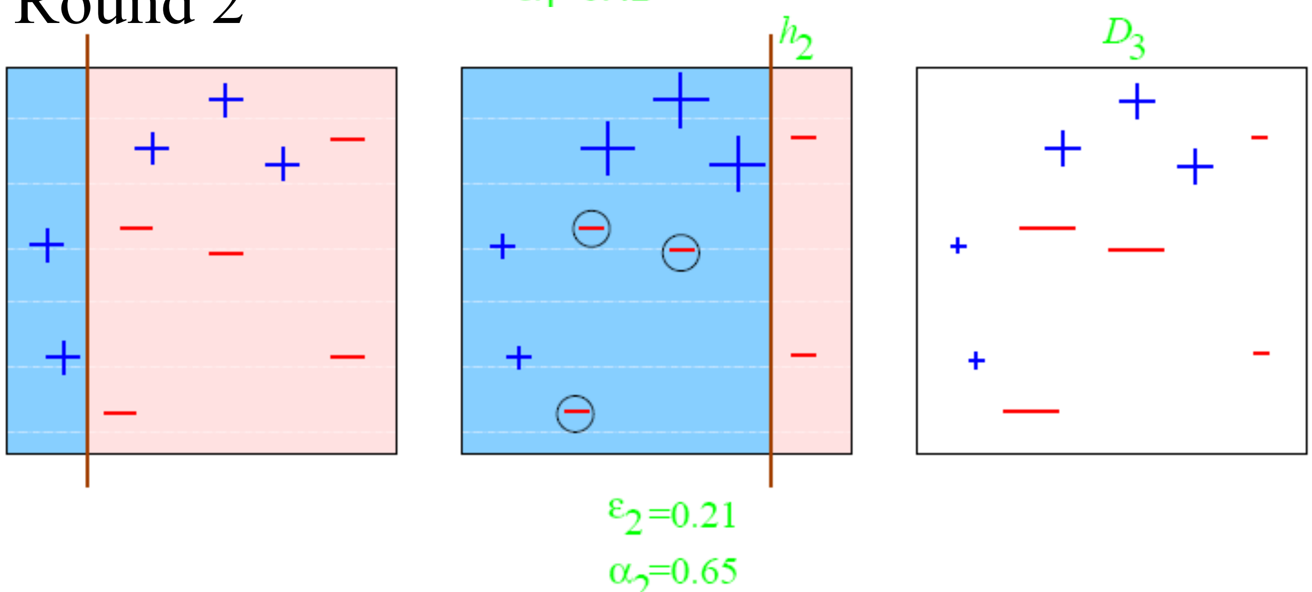
http://media.nips.cc/Conferences/2007/Tutorials/Slides/schapire-NIPS-07-tutorial.pdf

Rounds 1 and 2

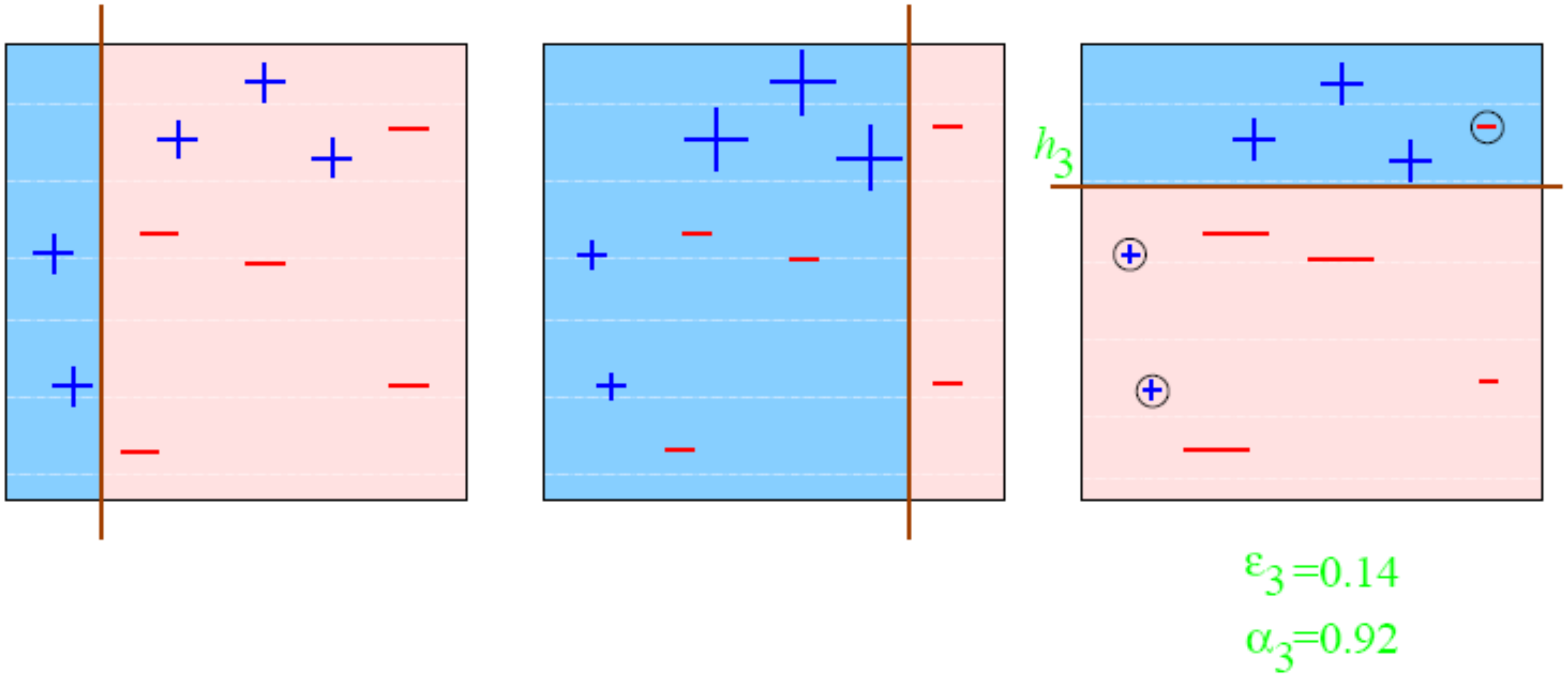
Round 1



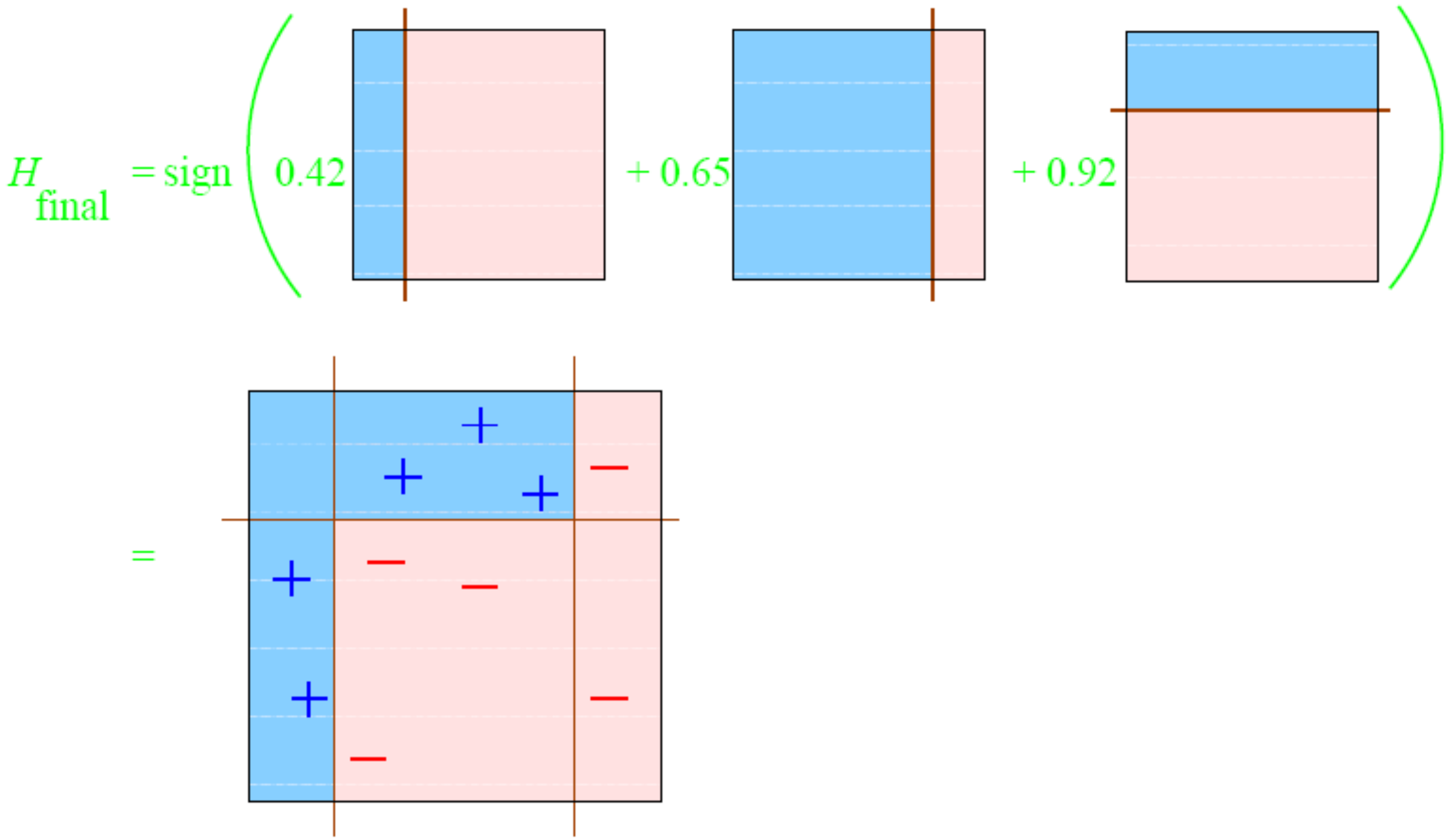
Round 2



Round 3



Final Classifier



Many Stumps win in the long run

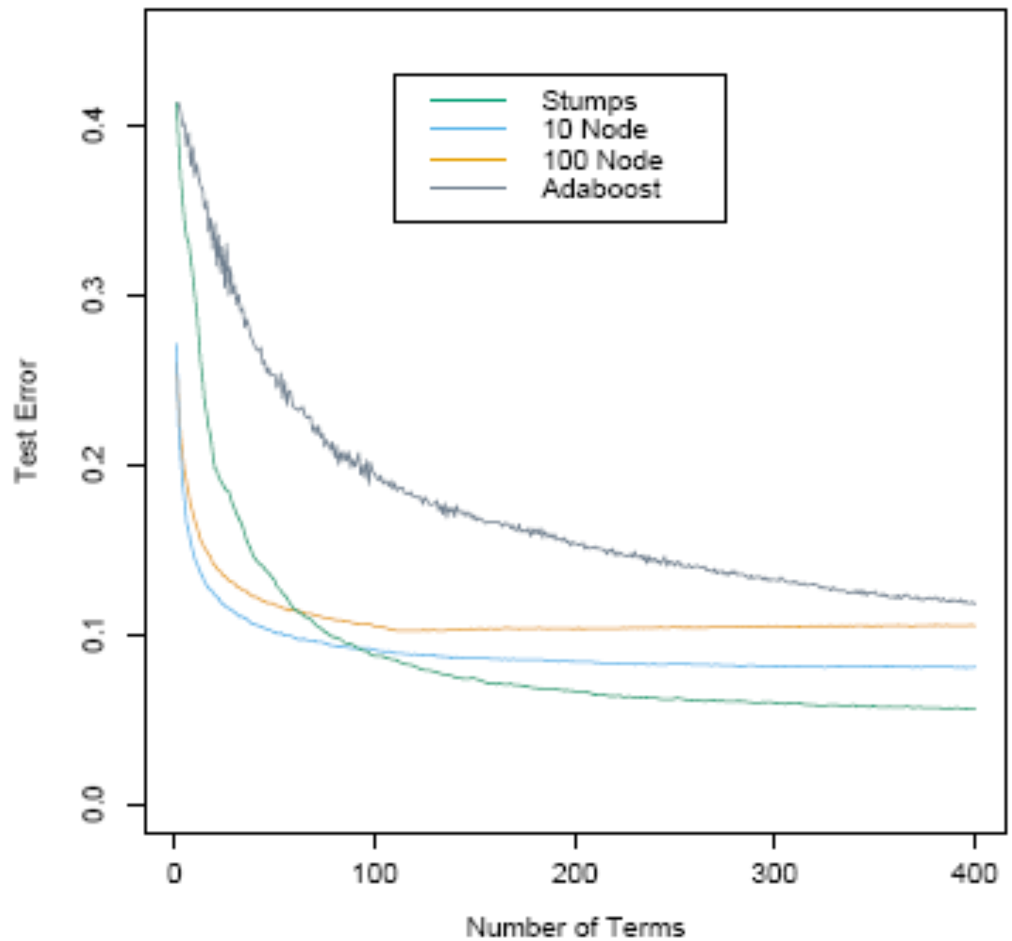


FIGURE 10.9. *Boosting with different sized trees, applied to the example (10.2) used in Figure 10.2. Since the generative model is additive, stumps perform the best. The boosting algorithm used the binomial deviance loss in Algorithm 10.3; shown for comparison is the AdaBoost Algorithm 10.1.*

Loss Function Comparison

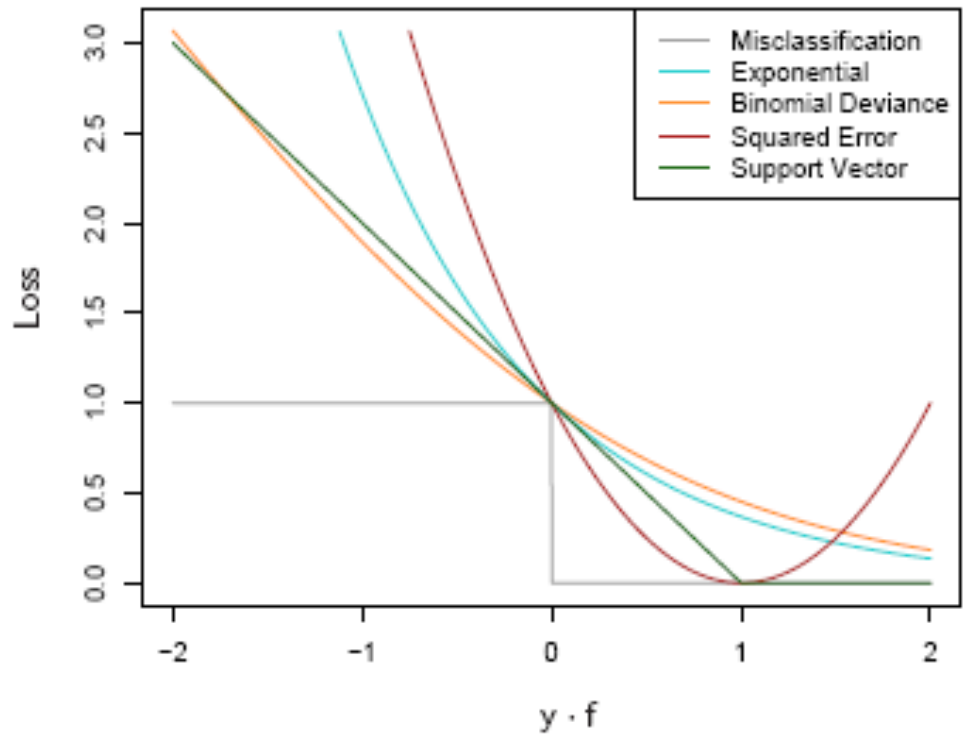


FIGURE 10.4. *Loss functions for two-class classification. The response is* $y = \pm 1$*; the prediction is* f*, with class prediction* $\text{sign}(f)$*. The losses are misclassification:* $I(\text{sign}(f) \neq y)$*; exponential:* $\exp(-yf)$*; binomial deviance:* $\log(1 + \exp(-2yf))$*; squared error:* $(y - f)^2$*; and support vector:* $(1 - yf)_+$ *(see Section 12.3). Each function has been scaled so that it passes through the point* $(0, 1)$.

- Additive model based on binomial deviance is more robust

Gradient Boosting

- See HTF Ch 10 for details and case studies
- **R Code: gbm** (Commercial: TreeNet)
  - Also in Scikit-learn
  - https://www.youtube.com/watch?v=IXZKgIsZRm0
- **Gradient descent in function space**
  - Less Greedy, more accurate, robust and interpretable than Adaboost
  - Can apply a variety of loss functions
  - Importance of variables (**for trees**): net information gain across all splits

Gradient descent in function space

TABLE 10.2. *Gradients for commonly used loss functions.*

Setting	Loss Function	$-\partial L(y_i, f(x_i))/\partial f(x_i)$
Regression	$\frac{1}{2}[y_i - f(x_i)]^2$	$y_i - f(x_i)$
Regression	$\|y_i - f(x_i)\|$	$\text{sign}[y_i - f(x_i)]$
Regression	Huber	$y_i - f(x_i)$ for $\|y_i - f(x_i)\| \leq \delta_m$ $\delta_m \text{sign}[y_i - f(x_i)]$ for $\|y_i - f(x_i)\| > \delta_m$ where $\delta_m = \alpha$th-quantile$\{\|y_i - f(x_i)\|\}$
Classification	Deviance	kth component: $I(y_i = \mathcal{G}_k) - p_k(x_i)$

Gradient Boosted (Decision) Trees (regression algorithm)*

Algorithm 10.3 *Gradient Tree Boosting Algorithm.*

1. Initialize $f_0(x) = \arg\min_\gamma \sum_{i=1}^{N} L(y_i, \gamma)$.
2. For $m = 1$ to M:
   (a) For $i = 1, 2, \ldots, N$ compute
   $$r_{im} = -\left[\frac{\partial L(y_i, f(x_i))}{\partial f(x_i)}\right]_{f=f_{m-1}}$$
   (b) Fit a regression tree to the targets r_{im} giving terminal regions R_{jm}, $j = 1, 2, \ldots, J_m$.
   (c) For $j = 1, 2, \ldots, J_m$ compute
   $$\gamma_{jm} = \arg\min_\gamma \sum_{x_i \in R_{jm}} L\left(y_i, f_{m-1}(x_i) + \gamma\right).$$
   (d) Update $f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} I(x \in R_{jm})$.
3. Output $\hat{f}(x) = f_M(x)$.

***Takeaway: Fits trees sequentially Using gradient boosting; Applies to regression/classification By using appropriate Loss fn*.**

GBDT can rank order features

- See HTF 10.14 for case studies

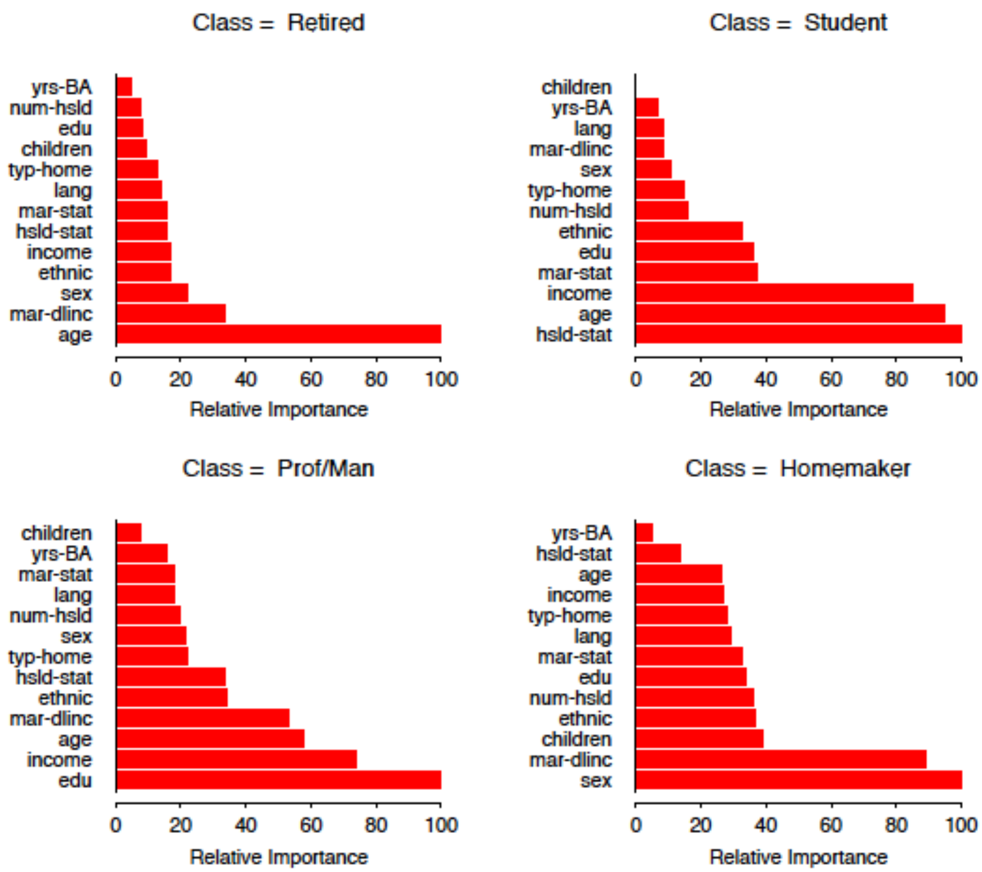
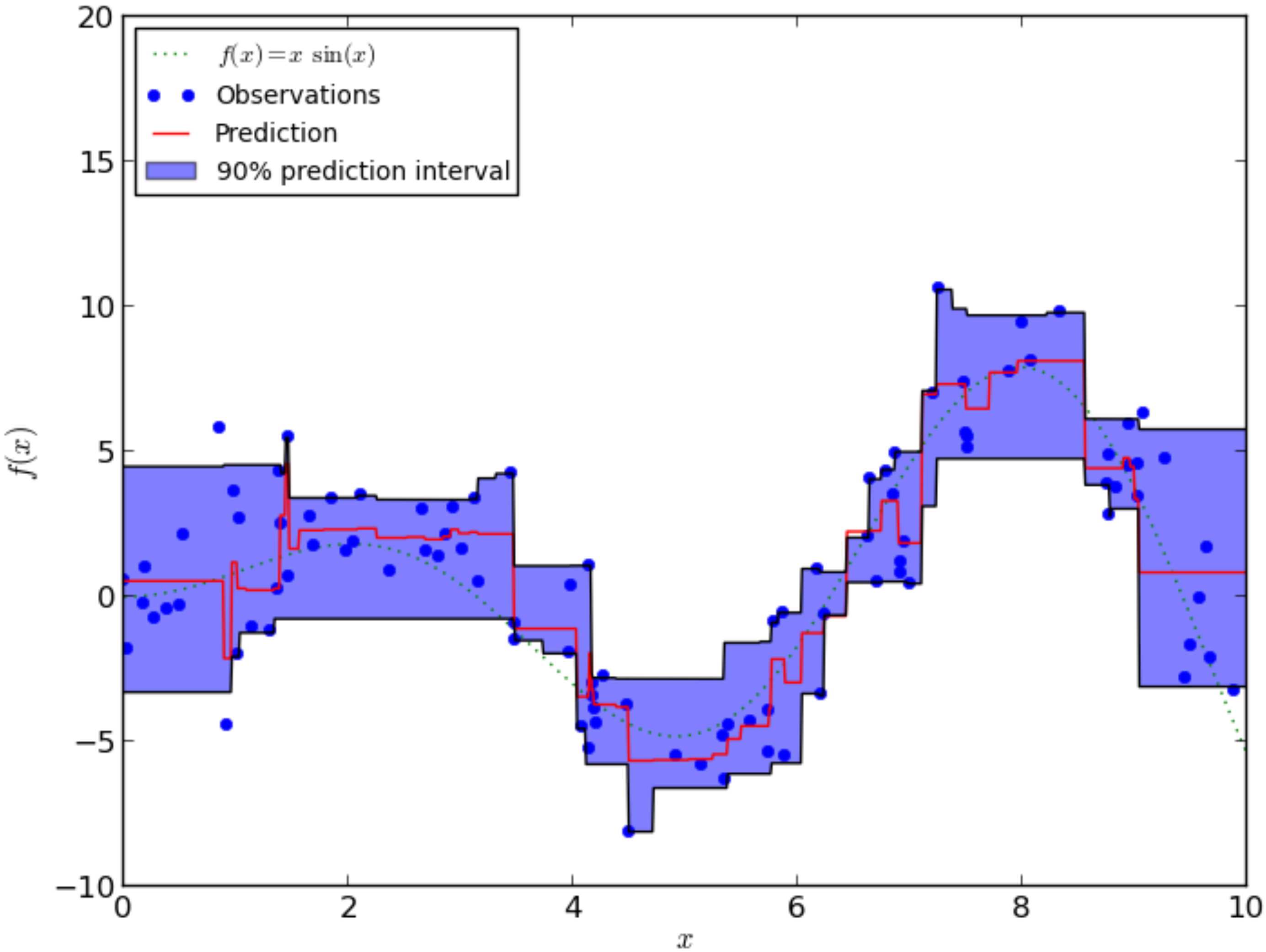


FIGURE 10.24. *Predictor variable importances separately for each of the four classes with lowest error rate for the demographics data.*

Occupation Prediction Example from HTF

Prediction Intervals

- http://scikit-learn.org/stable/auto_examples/ensemble/plot_gradient_boosting_quantile.html



Large Scale Boosting

- XGBoost: extreme Boosting
  - Boosts DTs as well as GLMs
    - Supports regression, classification, ranking and user defined objectives
  - Portable: desktop or cloud
  - Distributed
  - R and Python versions

  - https://xgboost.readthedocs.org/en/latest/
  - https://github.com/dmlc/xgboost
  - Needs tuning on several hyperparameters https://www.analyticsvidhya.com/blog/2016/03/complete-guide-parameter-tuning-xgboost-with-codes-python/

Summary of Committee Classifiers

- Variance reduction method
- Diversity is good (agree to disagree!)
- Good gains with little extra effort
- Provides estimate of decision confidence
  - Increased flexibility in accuracy-rejection rates
- "Standard"

Backups

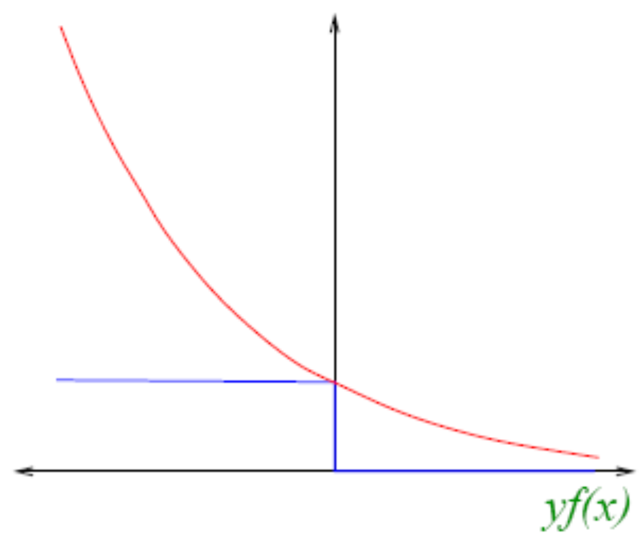
Boosting as a (Greedy) Additive Model

- (on a novel "exponential loss")
  - training error proof shows AdaBoost actually minimizes

$$\prod_t Z_t = \frac{1}{m}\sum_i \exp(-y_i f(x_i))$$

where $f(x) = \sum_t \alpha_t h_t(x)$

  - on each round, AdaBoost greedily chooses α_t and h_t to minimize loss
  - exponential loss is an upper bound on 0-1 (classification) loss
  - AdaBoost provably minimizes exponential loss



Early History

- Multi-class Winner-Take All: Selfridge's PANDEMONUIM (1958)
  - Ensembles of specialized demons
  - Hierarchy: Data, computational and cognitive demons
  - Decision : pick demon that "shouted the loudest"
    - Hill climbing; re-constituting useless demons, ….

- Nilsson's Committee Machine (1965)
  - Pick max of C linear discriminant functions:

$$g_i(\mathbf{X}) = \mathbf{W}_i^T \mathbf{X} + w_{i0}$$

Output Space Decomposition

Applying Multi-(binary) classifier systems for multi-class problems

- ECOC
- Hierarchical classifiers

History:

- Pandemonium, committee machine
  - "1 class vs. all others"
- Pairwise classification (how to combine?)
  - Limited
- Application specific solutions (80's)

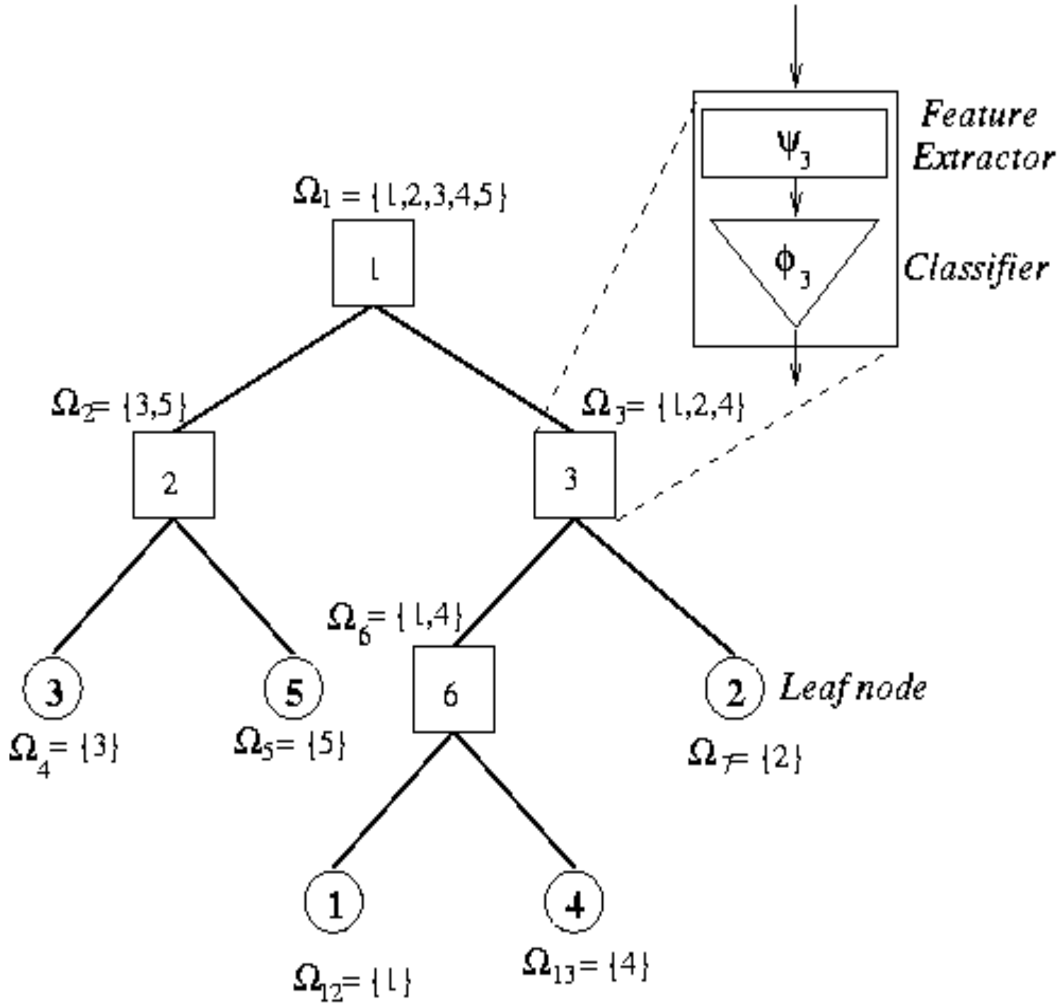
- ECOC: Error correcting output coding (Dietterich & Bakhiri, 95)

  +ve: # of meta-classifiers can be less; can tailor features

  -ve : groupings may be forced

- Desired: a general framework for natural grouping of classes
  - Hierarchical with variable resolution
  - Custom features

Binary Hierarchical Classifier



- Building the tree:
  - Bottom-Up
  - Top-Down
- Hard & soft variants
- Provides valuable domain knowledge
- Simplified feature extraction at each stage

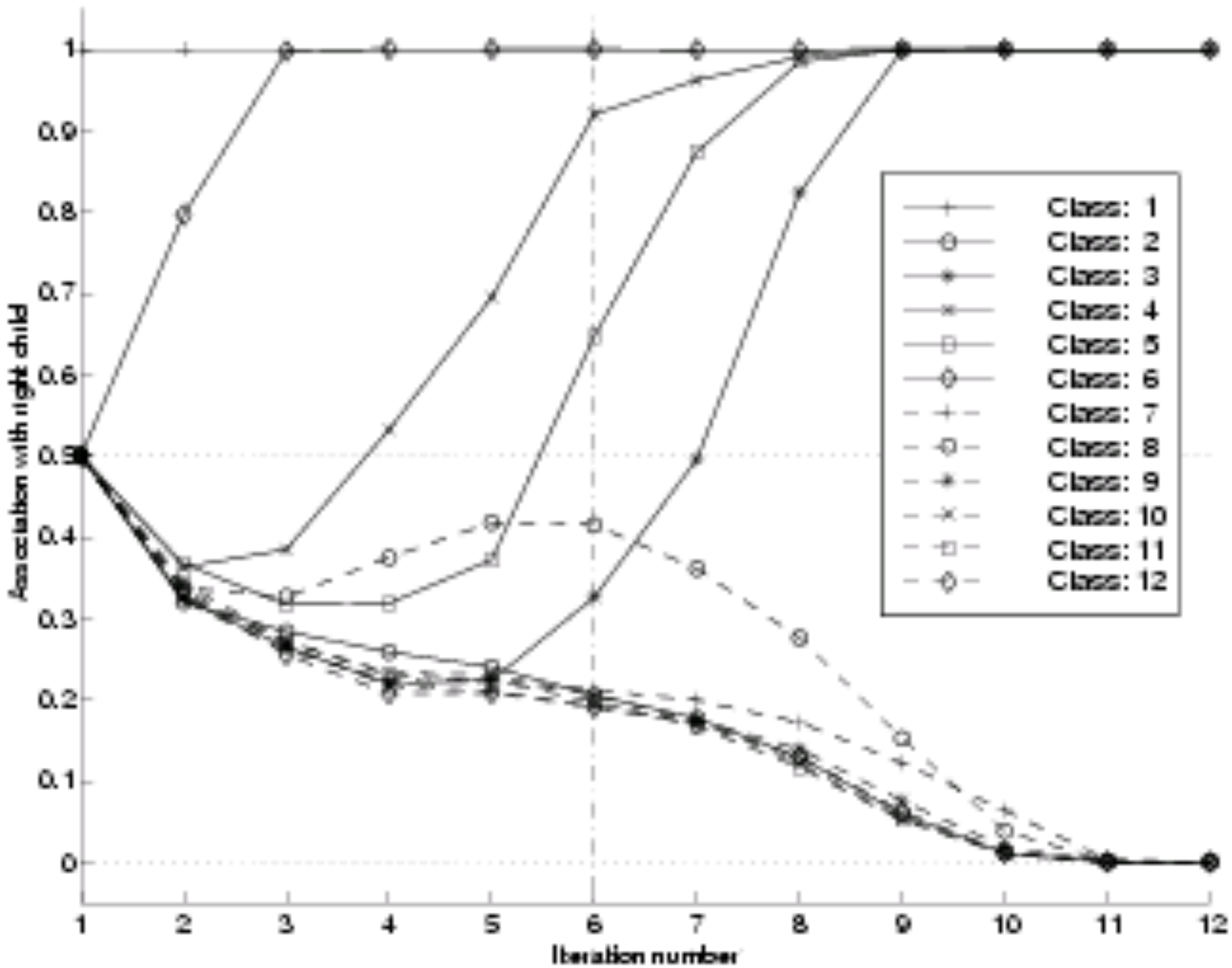
Hierarchical Grouping of Classes

- Top down: Solve 3 coupled problems
  - group classes into two meta-classes
  - design feaure extractor tailored for the 2 meta-classes (e.g. Fisher)
  - design the 2-metaclass classifier

- Solution using Deterministic Annealing :
  - Softly associate each class with both partitions
  - Compute/update the most discriminating features
  - Update associations;
    - For hard associations: also lower temperature
  - Recurse

  - Fast convergence, computation at macro-level

Evolution of Class Partitioning



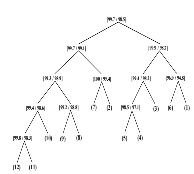
Assoc with Right Child -→

Iteration # -→

BHC-top down for AVIRIS (remote sensing)

- KSC; 183 band subset of 224 bands
- Class 1-8 Uplands; 9-12 Wetland

1. Scrub
2. Willow Swamp
3. Cab Palm Hammock
4. CP/Oak Hammock
5. Slash Pine
6. Oak/Broadleaf Hmk
7. Hardwood Swamp
8. Graminoid Marsh
9. Spartina Marsh
10. Cattail Marsh
11. Salt Marsh
12. Mud Flats



Motivation for Modular Networks

(Sharkey 97)

– More interpretable localized models (Divide and conquer)
– Incorporate prior knowledge
– Better modeling of inverse problems, discontinuous maps, switched time series, ..
– Future (localized) modifications
– Neurobiological plausibility

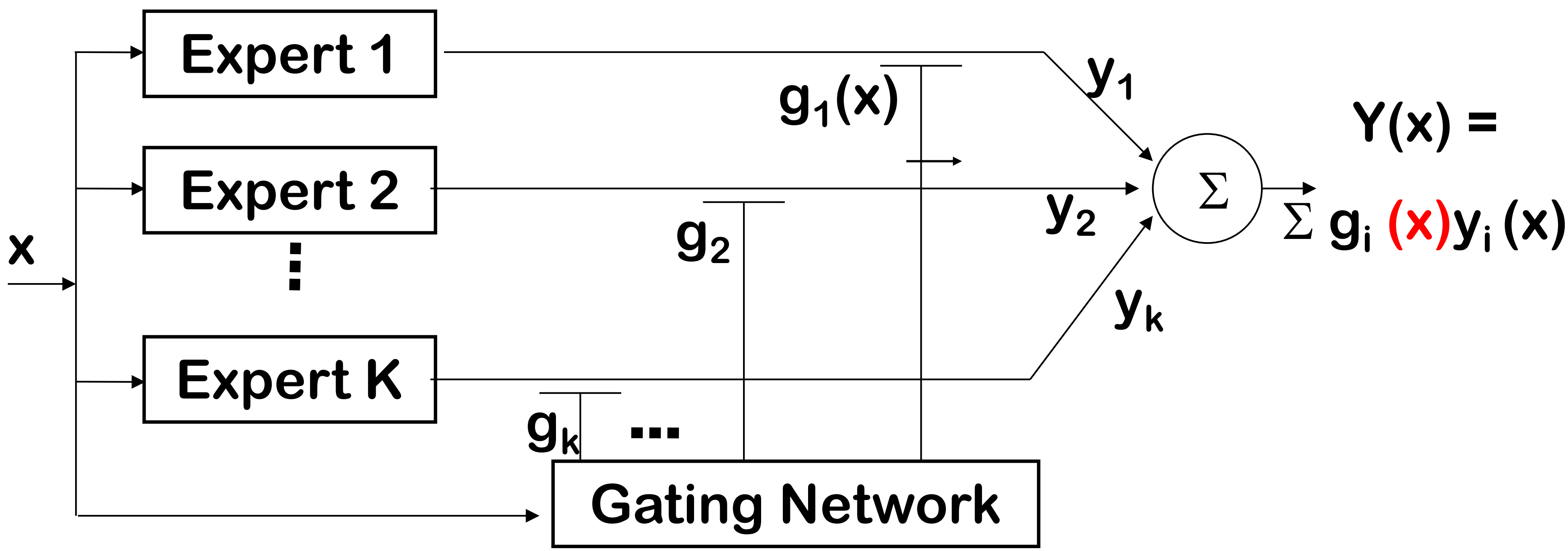
Varieties:

Cooperative, successive, supervisory,..

Automatic or explicit decomposition

Cop-operative Approach: Mixtures of Experts (MoE)

- Both $g_i(x)$' s and expert parameters adapted during training.



- Hierarchical versions possible

Generalizing MoE models

- Mixtures of X
  - X = HMMs, factor models, trees, principal components…
- State dependent gating networks
  - Sequence classification
- Mixture of Kalman Filters
  - Outperformed NASA's McGill filter bank!

W. S. Chaer, R. H. Bishop and J. Ghosh, "Hierarchical Adaptive Kalman Filtering for Interplanetary Orbit Determination", *IEEE Trans. on Aerospace and Electronic Systems*, 34(3), Aug 1998, pp. 883-896.

Beyond Mixtures of Experts

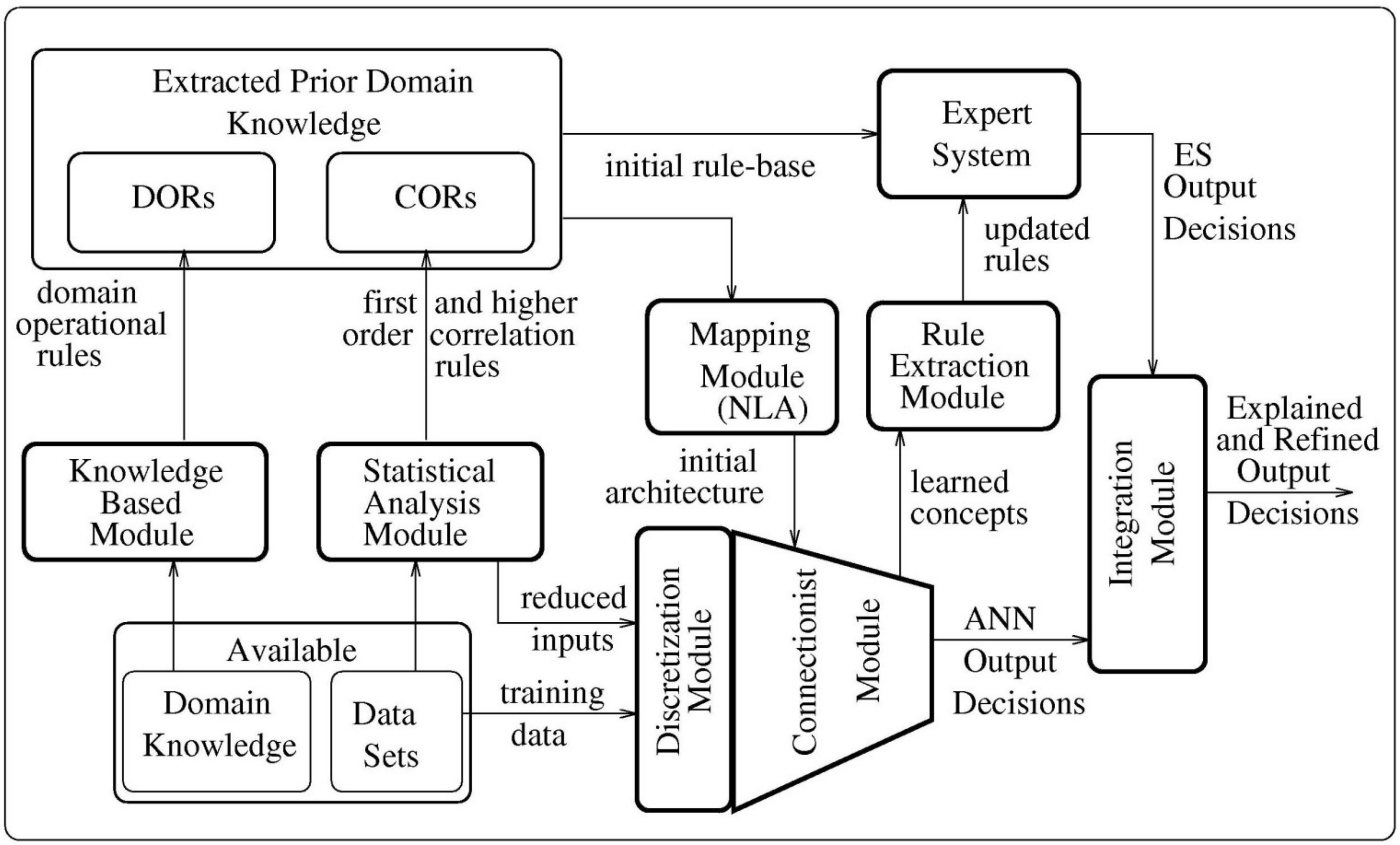
- Problems with soft-max based gating network

- Alternative: use normalized Gaussians
  - Structurally adaptive: add/delete experts
    - on-line learning versions
    - hard vs. soft switching; error bars, etc
  - Piaget's assimilation & accommodation

V. Ramamurti and J. Ghosh, "Structurally Adaptive Modular Networks for Non-Stationary Environments", IEEE Trans. Neural Networks, 10(1), Jan 1999, pp. 152-60.

Neuro-Symbolic Hybrids

- initial domain knowledge + follow-on data?
  - use hybrid (neural + symbolic) methods
  - Can extract refined domain knowledge!



Summary

Ensembles deliver!

- substantial gains for tough problem
    - Not much more extra effort
    - Bagging and boosting getting commercialized
    - Adds robustness to results
- Modular approaches suitable for niche problems

Output Space Decomposition

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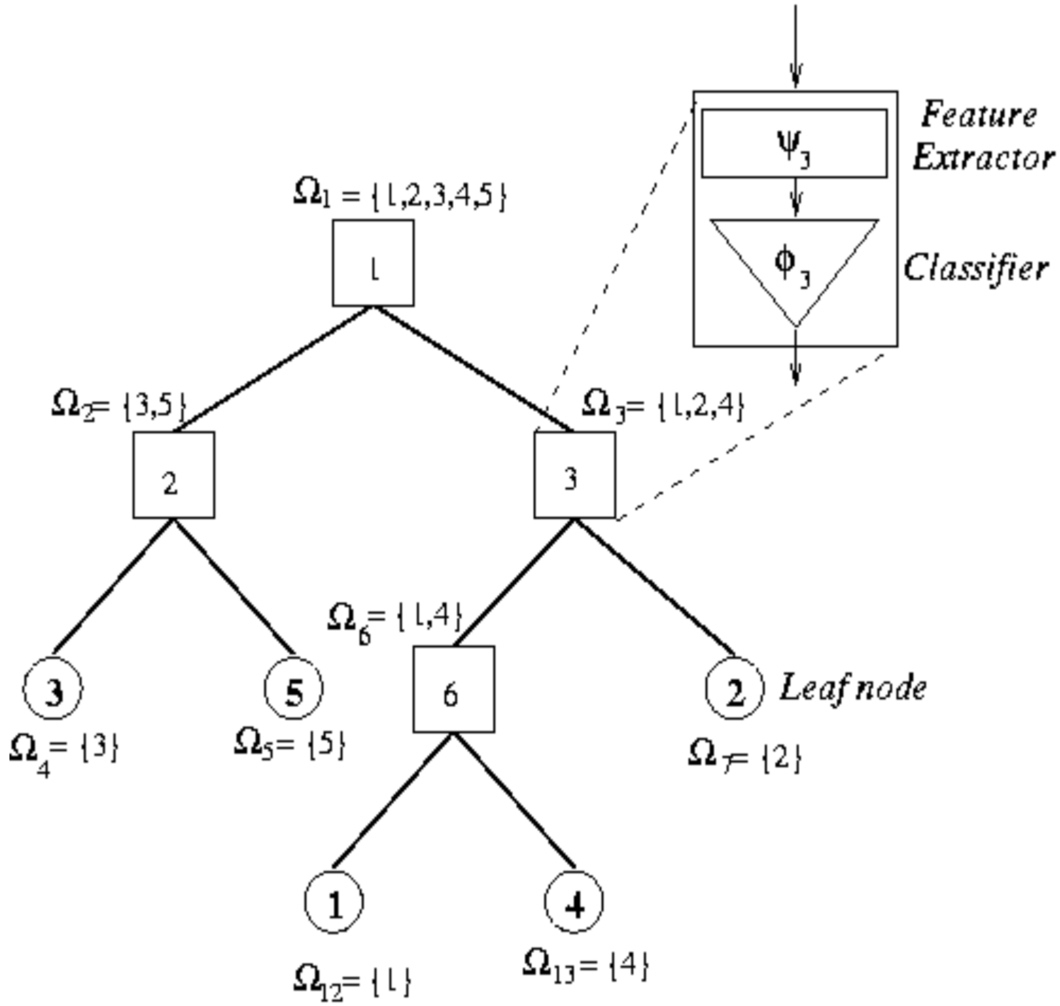
  - Custom features

Binary Hierarchical Classifier



- Building the tree:
  - Bottom-Up
  - Top-Down
- Hard & soft variants
- Provides valuable domain knowledge
- Simplified feature extraction at each stage

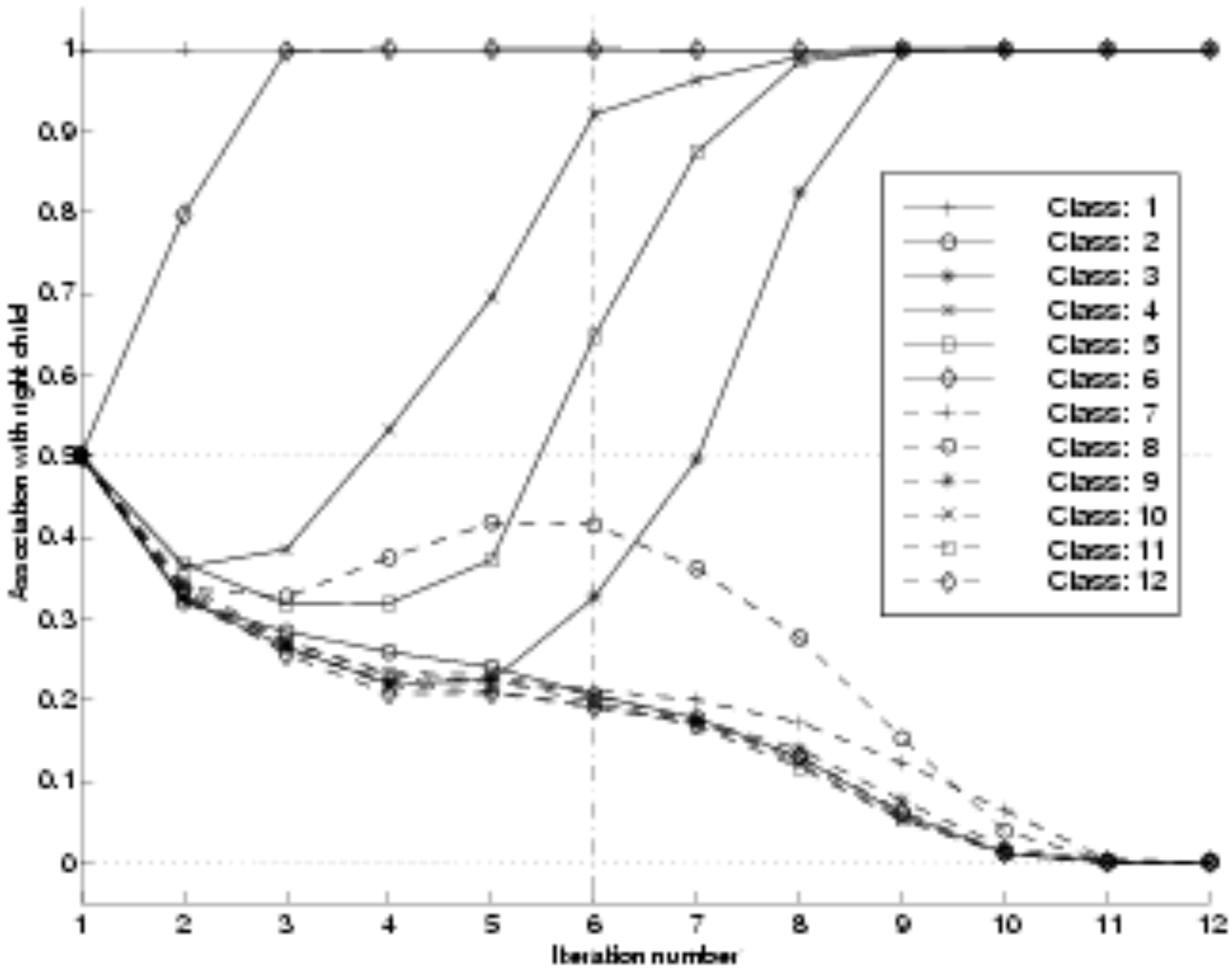
Hierarchical Grouping of Classes

- Top down: Solve 3 coupled problems
  - group classes into two meta-classes
  - design feaure extractor tailored for the 2 meta-classes (e.g. Fisher)
  - design the 2-metaclass classifier

- Solution using Deterministic Annealing :
  - Softly associate each class with both partitions
  - Compute/update the most discriminating features
  - Update associations;
    - For hard associations: also lower temperature
  - Recurse

  - Fast convergence, computation at macro-level

Evolution of Class Partitioning



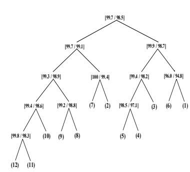
Assoc with Right Child -→

Iteration # -→

BHC-top down for AVIRIS (remote sensing)

- KSC; 183 band subset of 224 bands
- Class 1-8 Uplands; 9-12 Wetland

1. Scrub
2. Willow Swamp
3. Cab Palm Hammock
4. CP/Oak Hammock
5. Slash Pine
6. Oak/Broadleaf Hmk
7. Hardwood Swamp
8. Graminoid Marsh
9. Spartina Marsh
10. Cattail Marsh
11. Salt Marsh
12. Mud Flats



Motivation for Modular Networks

(Sharkey 97)

- More interpretable localized models (Divide and conquer)
- Incorporate prior knowledge
- Better modeling of inverse problems, discontinuous maps, switched time series, ..
- Future (localized) modifications
- Neurobiological plausibility

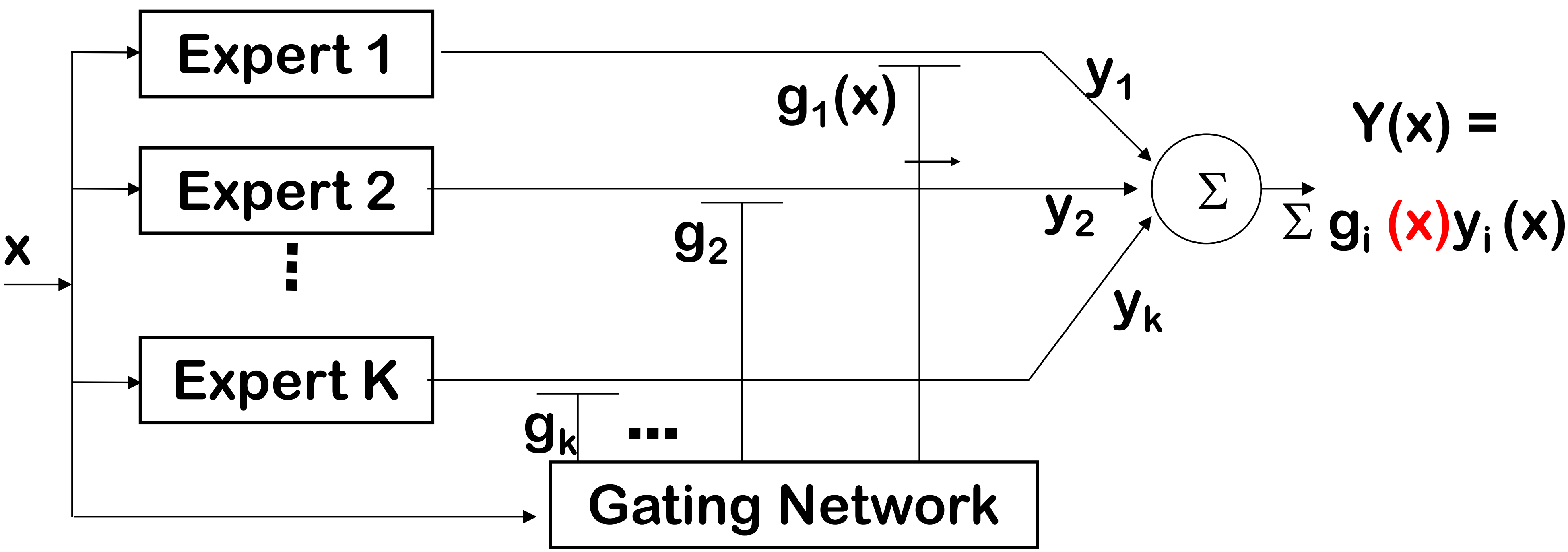
Varieties:

Cooperative, successive, supervisory,..

Automatic or explicit decomposition

Cop-operative Approach: Mixtures of Experts (MoE)

- Both $g_i(x)$' s and expert parameters adapted during training.



- Hierarchical versions possible

Generalizing MoE models

- Mixtures of X
  - X = HMMs, factor models, trees, principal components…
- State dependent gating networks
  - Sequence classification
- Mixture of Kalman Filters
  - Outperformed NASA's McGill filter bank!

W. S. Chaer, R. H. Bishop and J. Ghosh, "Hierarchical Adaptive Kalman Filtering for Interplanetary Orbit Determination", *IEEE Trans. on Aerospace and Electronic Systems*, 34(3), Aug 1998, pp. 883-896.

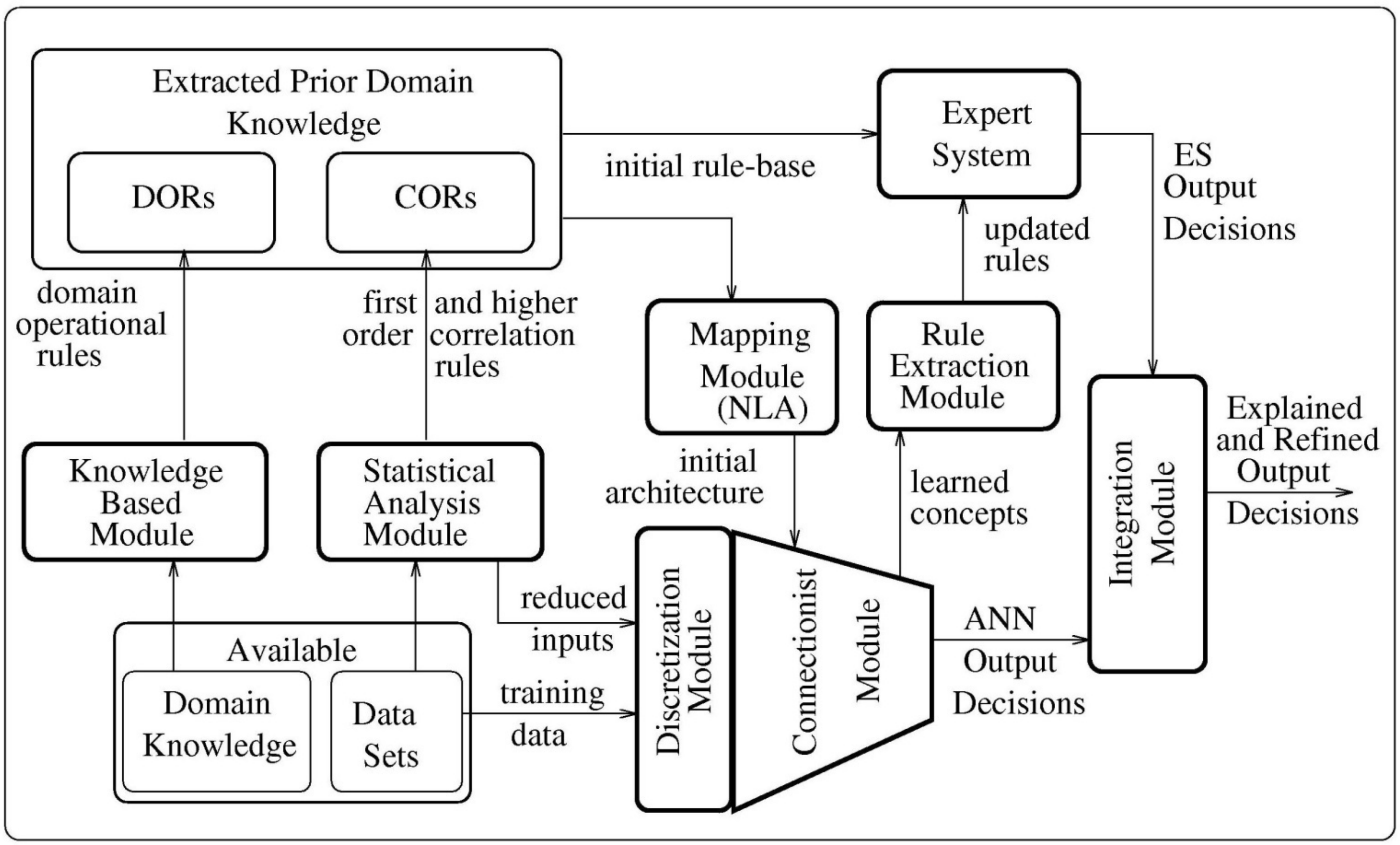
Beyond Mixtures of Experts

- Problems with soft-max based gating network
- Alternative: use normalized Gaussians
  - Structurally adaptive: add/delete experts
    - on-line learning versions
    - hard vs. soft switching; error bars, etc
  - Piaget's assimilation & accommodation

V. Ramamurti and J. Ghosh, "Structurally Adaptive Modular Networks for Non-Stationary Environments", IEEE Trans. Neural Networks, 10(1), Jan 1999, pp. 152-60.

Neuro-Symbolic Hybrids

- initial domain knowledge + follow-on data?
  - use hybrid (neural + symbolic) methods
  - Can extract refined domain knowledge!



Summary

Ensembles deliver!

- substantial gains for tough problem
    - Not much more extra effort
    - Bagging and boosting getting commercialized
    - Adds robustness to results
- Modular approaches suitable for niche problems