Master of Technology in Knowledge Engineering

Advanced Modeling Topics in Data Mining

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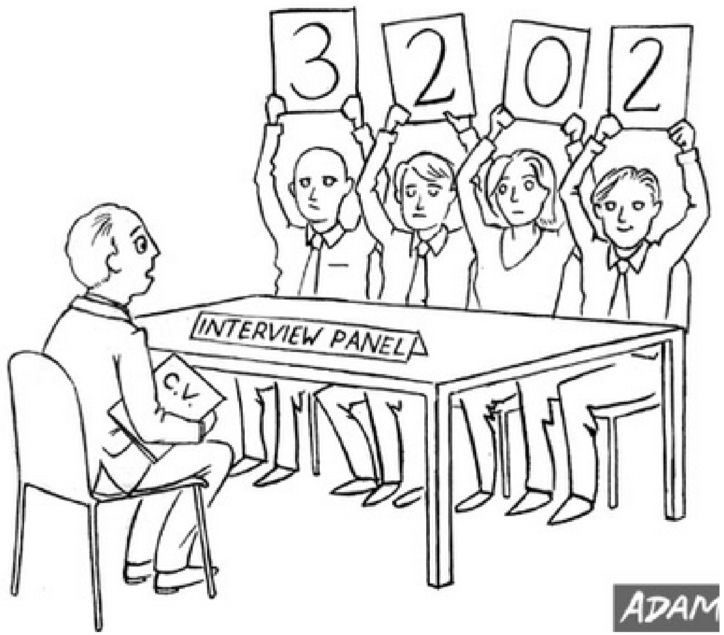
Agenda for the Day

- To introduce a selection of advanced data mining techniques and topics, in particular:
  – Ensemble Methods
    - Bagging
    - Random Forests
    - Boosting
  – Multiple Classifier Systems

- Workshop

What are Ensembles?

- Ensembles are committees of multiple models
- Each model makes a prediction or "vote"
- Final prediction is average/majority of votes
  - Majority vote for classification (class prediction)
  - Average prediction for regression problems (value prediction)



- What benefits does this bring?
- Why not just train one smart model?

Motivation

- Assume one model and 5 test cases

Truth	**1**	**0**	**1**	**1**	**0**	**Accuracy**
Model 1	1	0	**0**	1	**1**	60%

Motivation

- Add another 4 models, each with same accuracy, but with variance (models do not give identical predictions)

Truth	**1**	**0**	**1**	**1**	**0**	**Accuracy**
Model 1	1	0	**0**	1	**1**	60%
Model 2	**0**	**1**	1	1	0	60%
Model 3	**0**	0	1	**0**	0	60%
Model 4	1	**1**	1	1	**1**	60%
Model 5	1	0	**0**	**0**	0	60%
Vote 1-5	**1**	**0**	**1**	**1**	**0**	**100%**

- No one model is very accurate, learns everything
- Performance of ensemble outperforms individuals
- Usually more reliable/robust than individual models

What makes a good ensemble?

- The term *ensemble* is usually reserved for methods that generate multiple hypotheses using the same base learner*

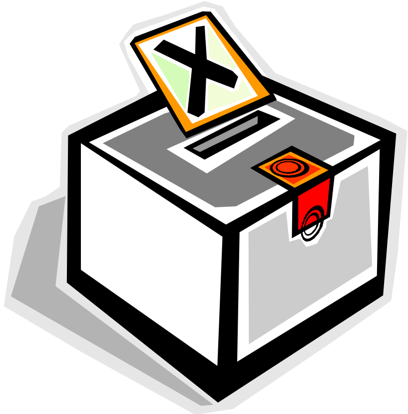
"A necessary and sufficient condition for an ensemble of classifiers to be more accurate than any of its individual members is if the classifiers are accurate and diverse"

-- Tom Dietterich (2000)

(*the broader term of *multiple classifier systems* covers ensembles that do not use the same base learner)

How to get suitable diverse models?

- *Ensembles* tend to yield better results when there is a significant diversity among the models
- Bagging is one way of introducing diversity
  - Train many models with different random samples
  - Usually applied to decision trees, but can be used with any method

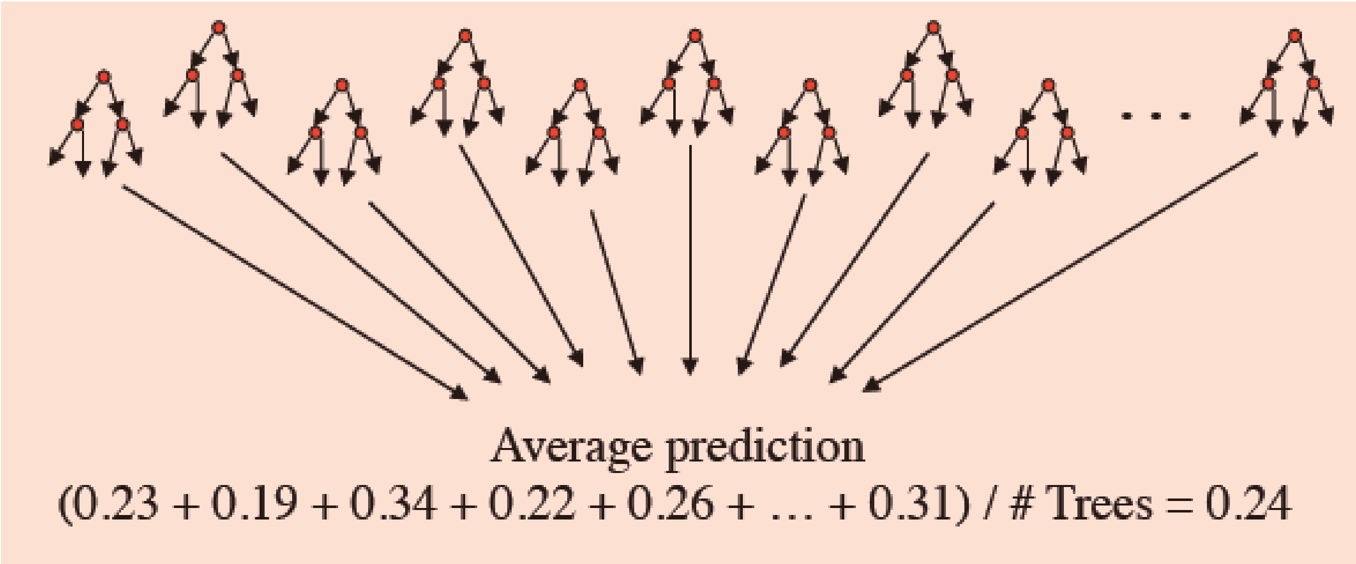


When using bagging, each learned model has a vote of equal value

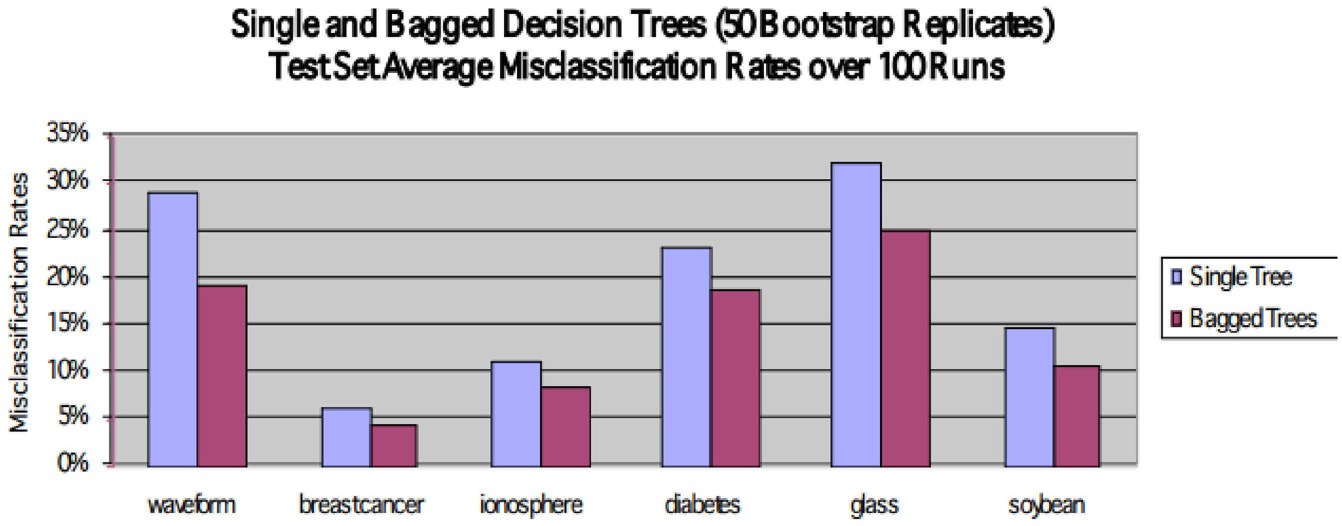
- Where do we get many different random samples?

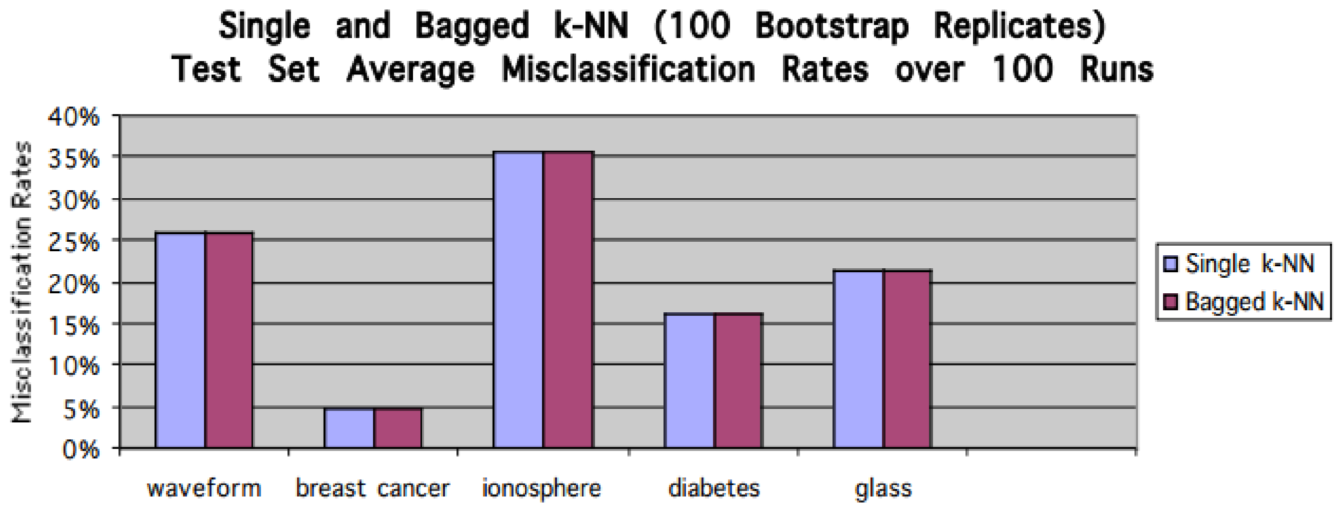
Bagging: Bootstrap Aggregating

- Draw N (say 100) bootstrap samples (sampling with replacement) from the training data, Train decision trees on each sample
- Algorithm:
  - Randomly draw 67% (say, two thirds) of the training data
  - Train a tree on this sample
  - Repeat this N times to get N trees
- Take the un-weighted average prediction of all trees



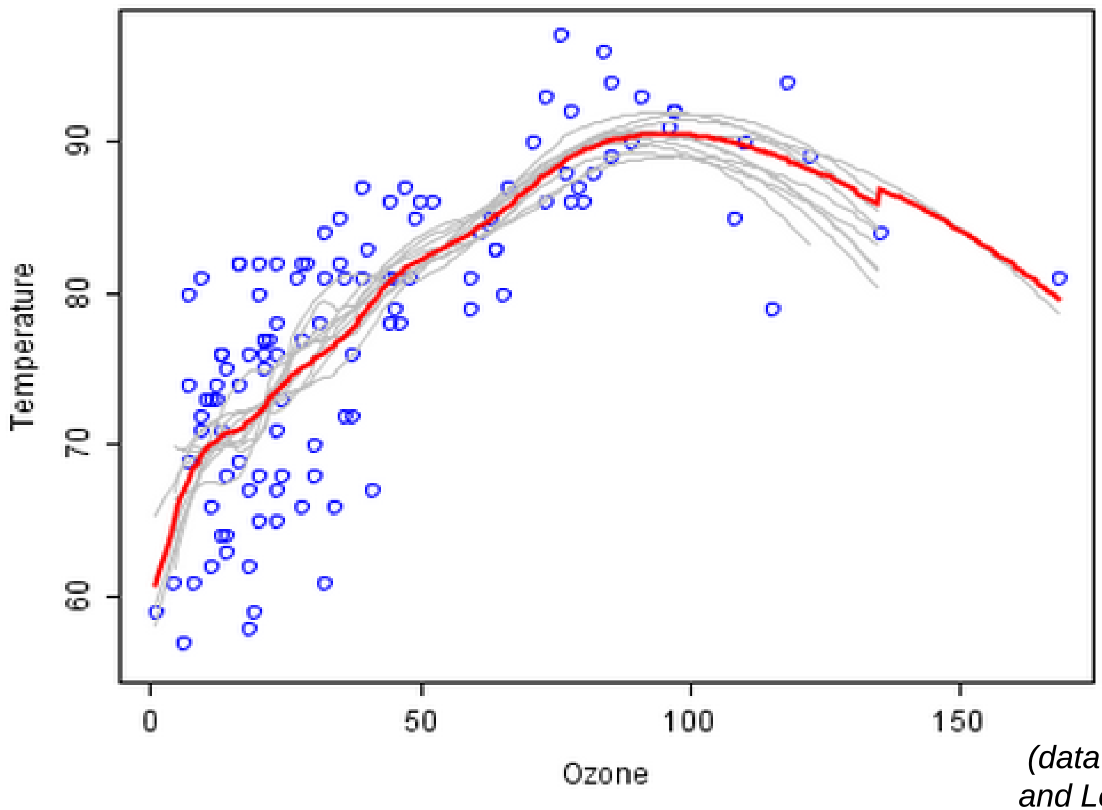
Examples of Bagging (Breiman, 1996)





Examples of Bagging

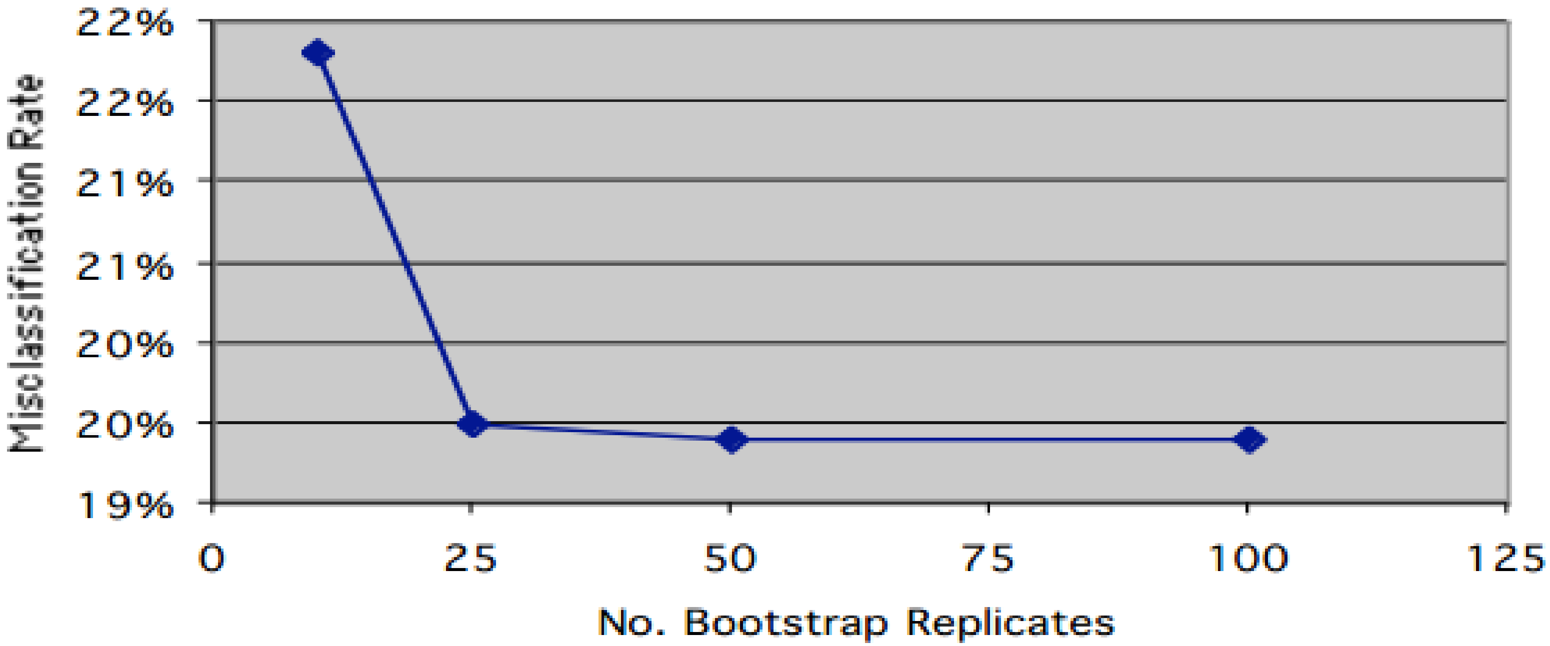
- Ensemble of 10 regression smoothers built from 10 bootstrap samples, each drawing 100 training data.



(data from Rousseeuw and Leroy (1986)).

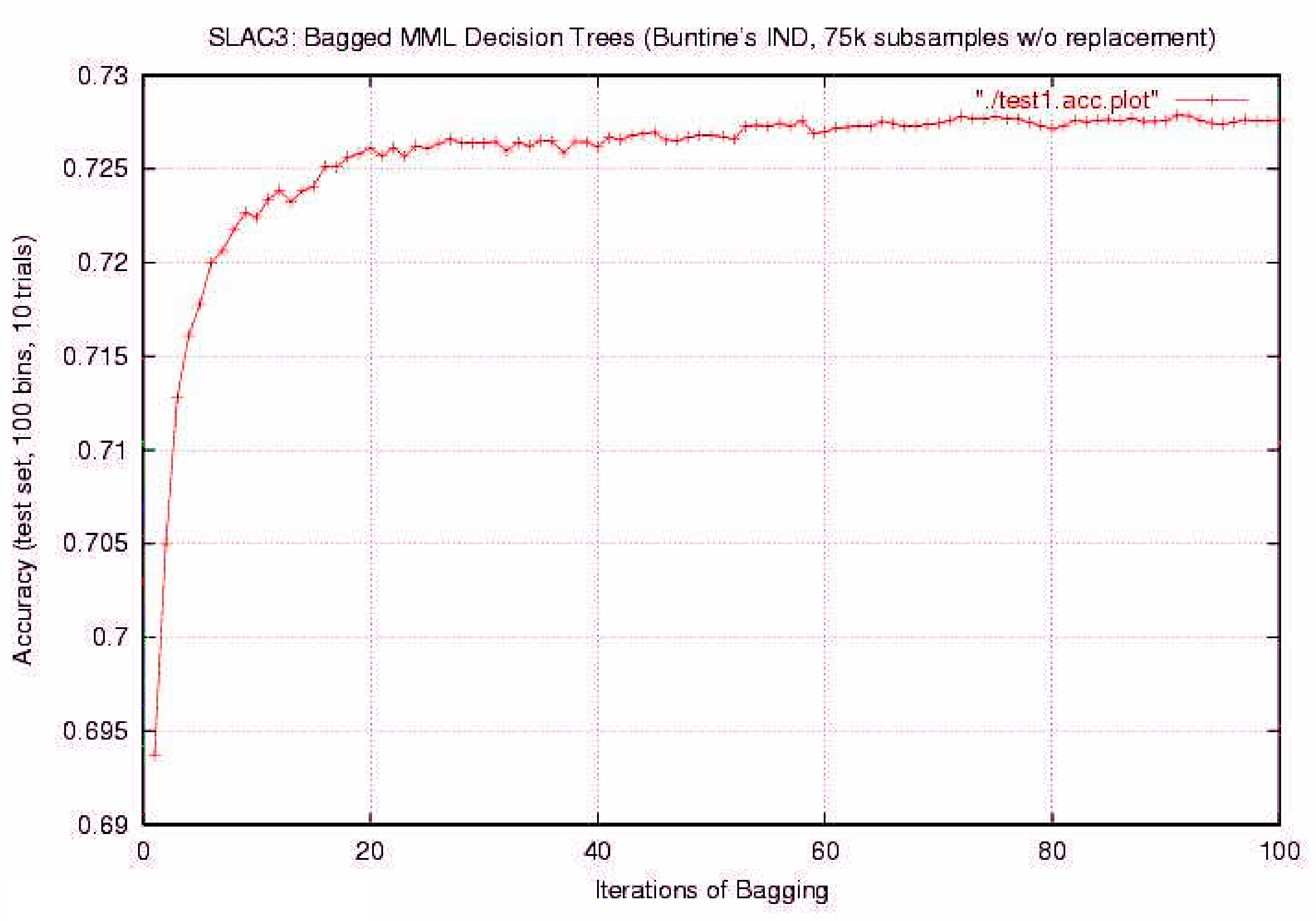
How Many Bagged Models Are Required?

- Example from the soybean data set , Breiman, 1996:



- Depends on data and problem, but generally, < 50 models should work well and often < 25 is adequate

How Many Bagged Models Are Required?



Why does it work? Model Error Reduction

- Assume we build a prediction model $\hat{f}(X)$ (using regression or decision trees etc.) to estimate a function $f(X)$ where X is the set of input variables and Y is the variable to be predicted
- Then the expected squared prediction error at point x is:

$$Err(x) = E\left[(Y - \hat{f}(x))^2\right]$$

- We can decompose this into 3 components

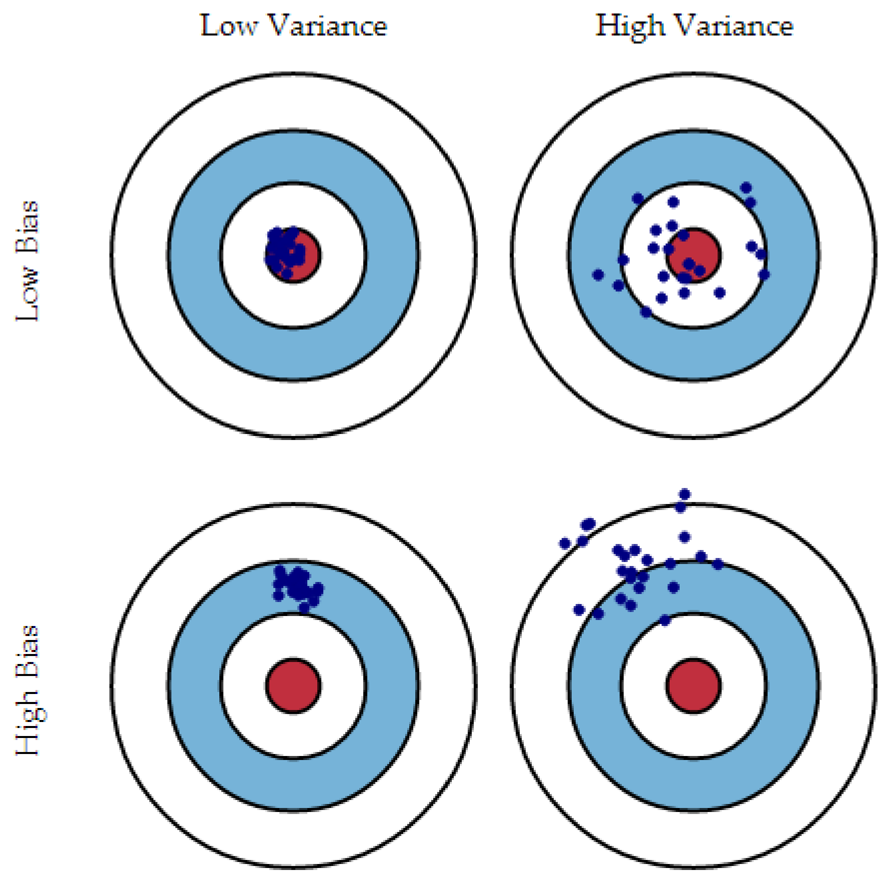
$$Err(x) = \left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

$$Err(x) = \mathrm{Bias}^2 + \mathrm{Variance} + \underbrace{\mathrm{Irreducible\ Error}}_{}$$

Noise, cannot be reduced by the model

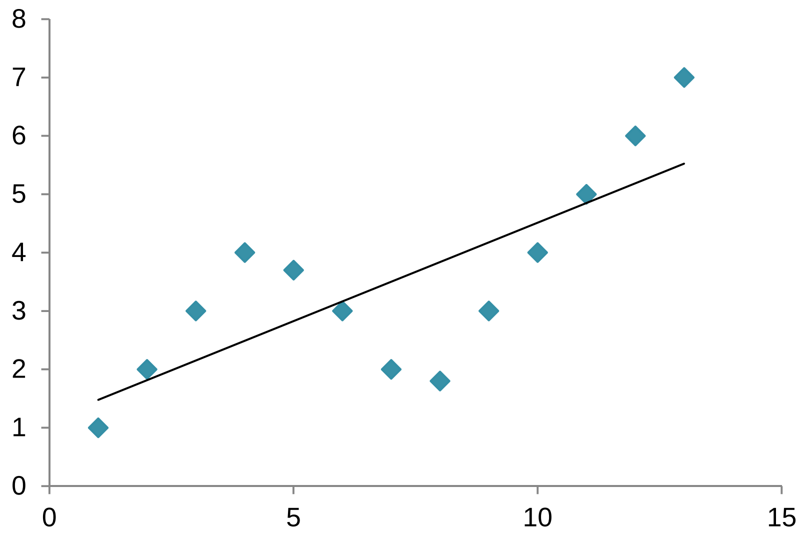
Model Error: Bias versus Variance

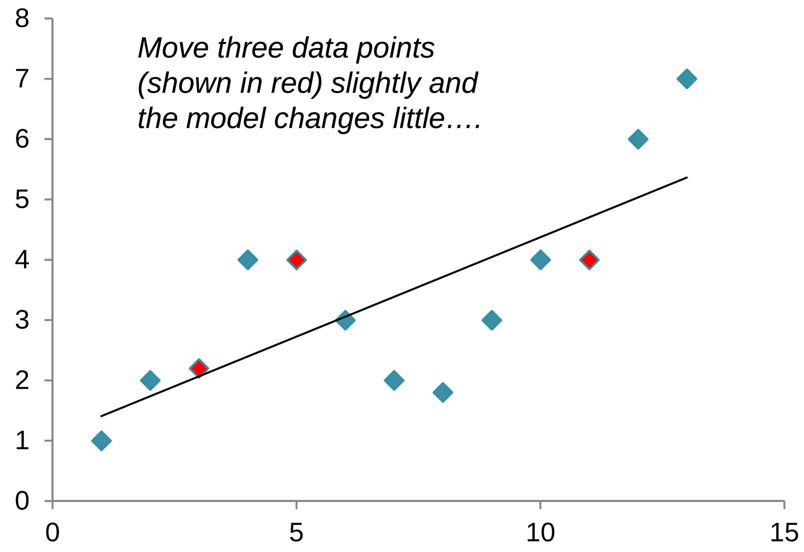
- **Assume**
  - You sample a population N times and build a model from each sample, then…
- **Error due to Bias**:
  - The difference between the expected (or average) prediction of the model and the correct value
- **Error due to Variance**:
  - The variability of the model prediction for a given data point



Model Error: Bias versus Variance

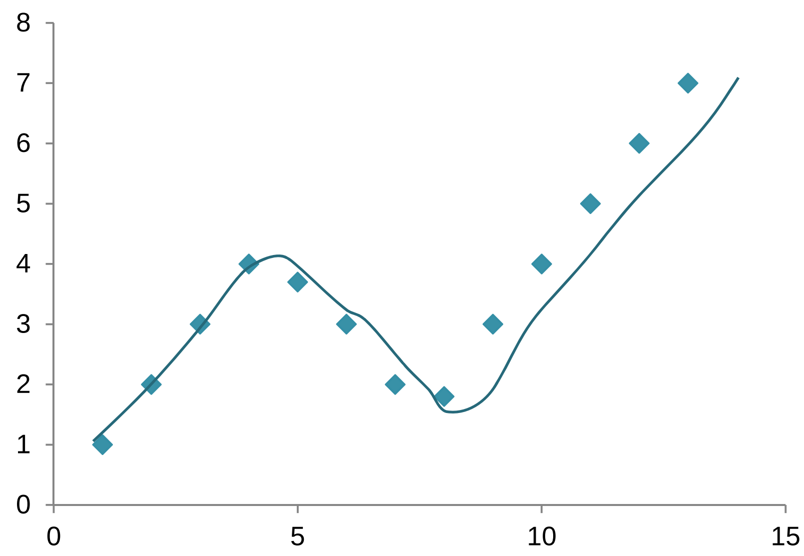
- Models that under-fit the data tend to have:
  - High bias ~ the model doesn't fit the training data very well
  - Low variance – removing/changing a few training data points won't change the model or predictions much

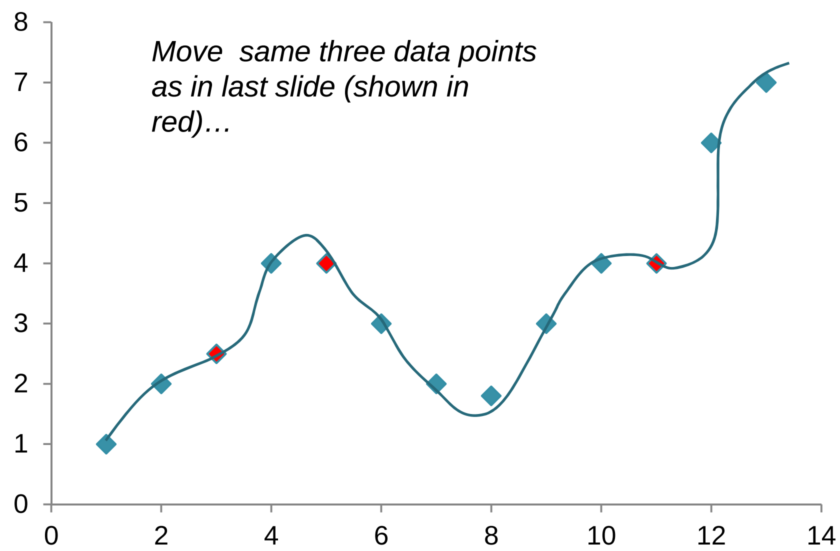




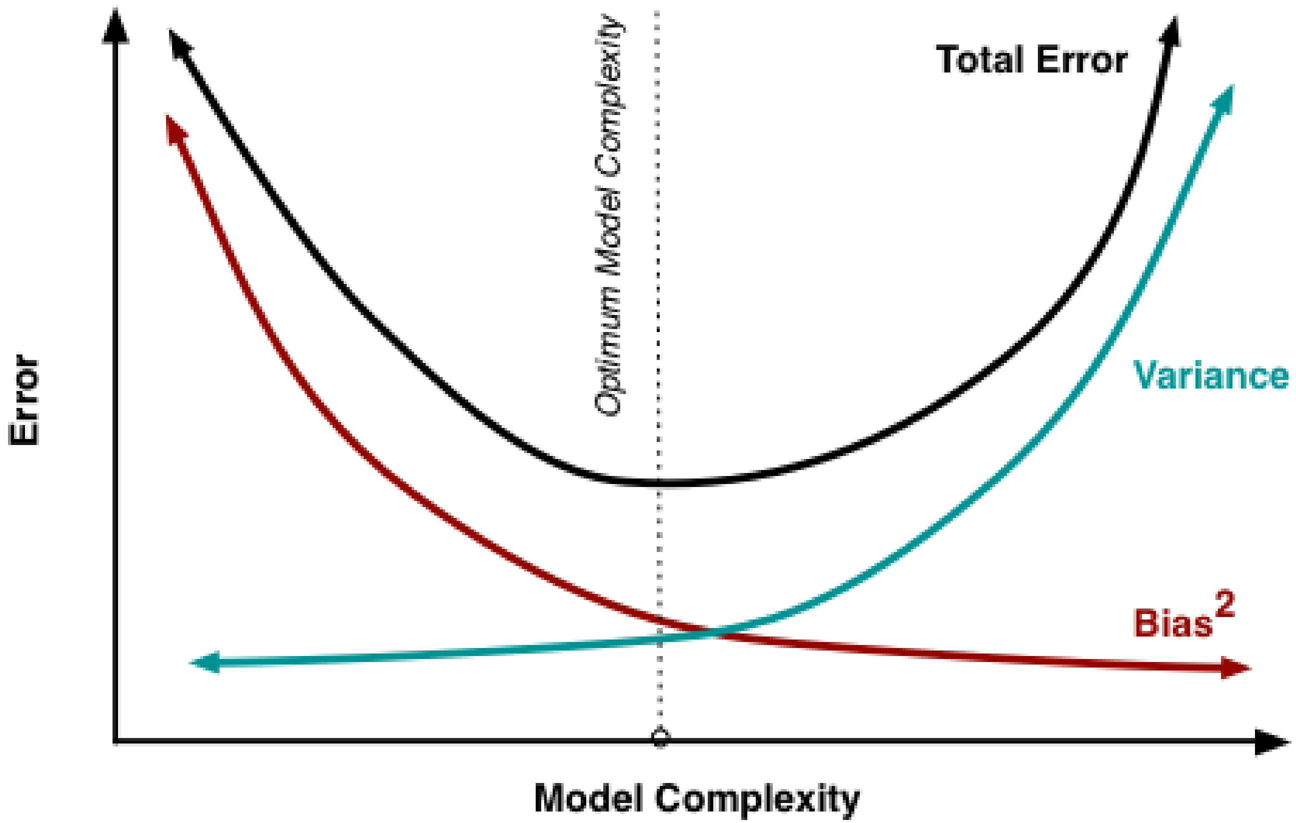
Model Error: Bias versus Variance

- Models that over-fit the data tend to have:
  - Low bias ~ the model fits the training data very well
  - High variance – removing/changing a few training data points can change the model and hence the predictions a lot





Tradeoff between Bias and Variance



Tradeoff between Bias and Variance

- Reducing bias & variance is important for prediction accuracy
- Tradeoff:
  - bias vs. variance
  - high complexity models vs. low complexity models
  - most errors due to over-fitting vs. most errors due to under-fitting
  - choice: smart twitchy (sensitive) models vs. less smart but stable models
- Clearly we want smart models, but…
  - Can we reduce variance without increasing bias?
  - Can we reduce over-fitting without under-fitting?

YES!

Reduce Variance Without Increasing Bias

- Averaging reduces variance:

$$Var(\overline{X}) = \frac{Var(X)}{N}$$

- Average models to reduce model variance
- For large N, residual model error mainly due to bias!
- In practice:
  - models are correlated, so reduction is smaller than 1/N
  - variance of models trained on fewer training cases is usually larger
  - only works with some learning methods: very stable learning methods have such low variance to begin with, that bagging does not help much.

Can Bagging Hurt?

- Each base classifier is trained on less data
  - E.g. only about 67% of the data points are in any one bootstrap sample
- If data is poor, then losing this much data can hurt accuracy
- Bagging usually helps, but sometimes not much…

Other ways to create Model Diversity

- Manipulating the training data (e.g. bagging)
- Manipulating the input features
- Varying the classifier type, architecture

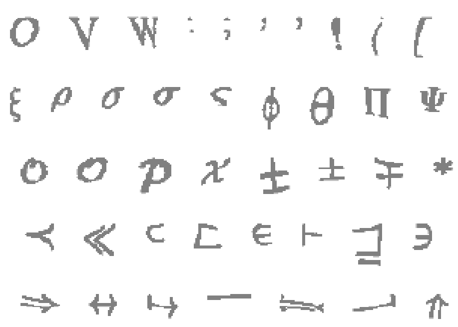
Random Forests

- Draw *1000*+ bootstrap samples of data
- ***Draw random sample of available features at each tree split***
  - Randomisation (hence model diversity) now occurs in two places: Random sampling of *training data* + Random sampling of *feature set*
  - Training speed increases due to less computation at each tree split (less features to evaluate the splitting cost function for)
- Train trees on each sample/attribute set -> *1000*+ trees
- Use un-weighted voting to get final prediction (as with bagging)

Random Forests

- Usually works better than bagging
  - robust to noise, easy to use, surprisingly high accuracy
  - but.. lots of trees means hard to interpret (becomes a black box)
- Variance of RF trees is higher than Bagged Trees
  - typically needs 10X as many trees
  - trees should be (generally) unpruned (to encourage diversity)
  - RF needs 100's to 1000's
- Extra parameter to tune: p(feat)
  - probability of getting to use feature at each split
  - fortunately, usually not too sensitive
  - Breiman suggests SQRT(N), N: total number of features
- Unlike Bagging and Boosting, RF is for trees only
- Microsoft's Kinect (3D motion sensor) uses random forests

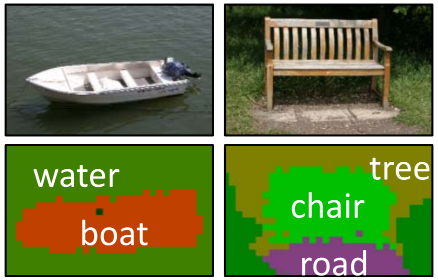
Random Forests in Vision



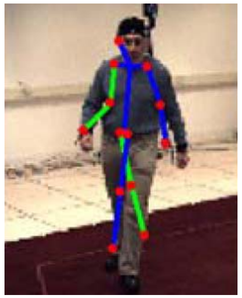
[Amit & Geman, 97]
digit recognition

[Lepetit *et al.*, 06]
keypoint recognition

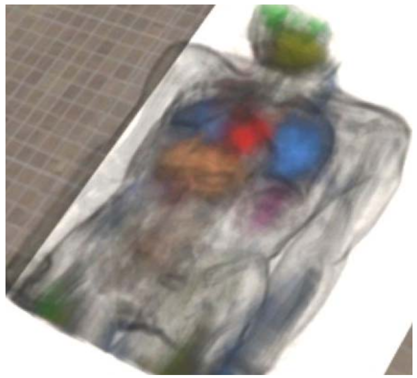
[Moosmann *et al.*, 06]
visual word clustering



[Shotton *et al.*, 08]
object segmentation



[Rogez *et al.*, 08]
pose estimation

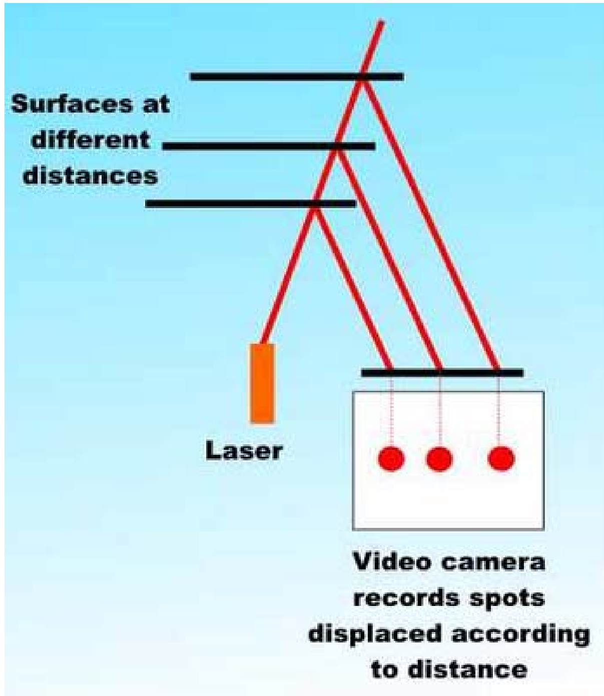


[Criminisi *et al.*, 09]
organ detection

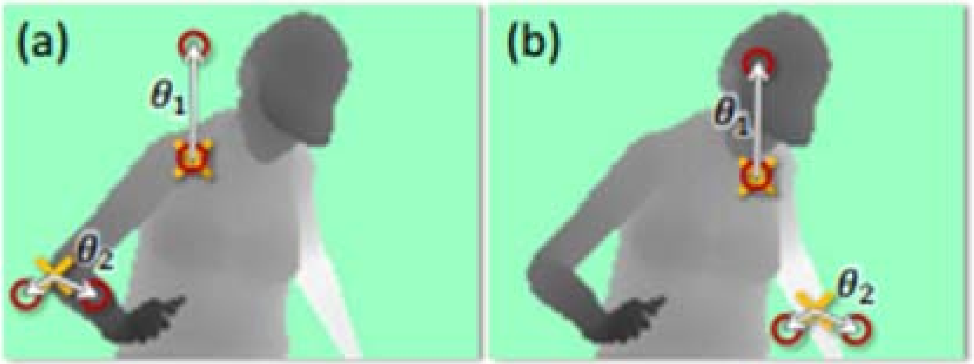
(Among many others...)

Kinect’s Decision Forest

- Step1: Generate a 3D image
  - Kinect uses "structured light“ ~ If you have a light source offset from a detector by a small distance then the projected spot of light is shifted according to the distance it is reflected back from.



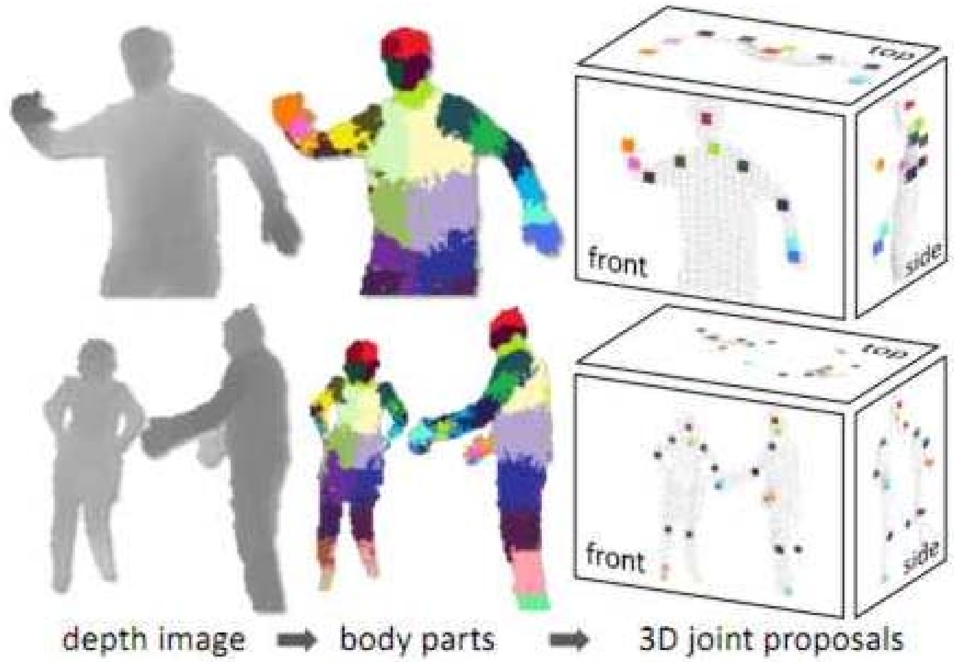
- Step2: Compute Features
  - Compute the difference in depth (z) to two pixels that are close together in (x,y). If difference is small then they likely belong to same object. Repeat many times.



Kinect's Decision Forest

- Step3: Build Forest
  - Each tree was trained on features that were pre-labeled with the target body parts.
  - Training just 3 trees using 1 million test images took a day using a 1000 core cluster.
  - The trained classifiers assign a probably of a pixel being in each body part

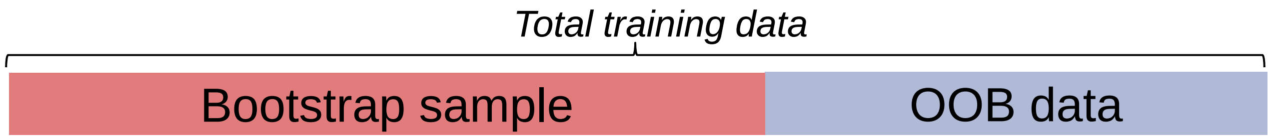
- Step4: Execute the Forest
  - Picks areas of maximum probability for each body part type.



http://www.youtube.com/watch?v=HNkbG3KsY84

Testing Random Forests

- No need for separate test set
- Method:
  - Test each tree against the data left over after the bootstrap sample was taken; this is called the OOB (out-of-bag) data

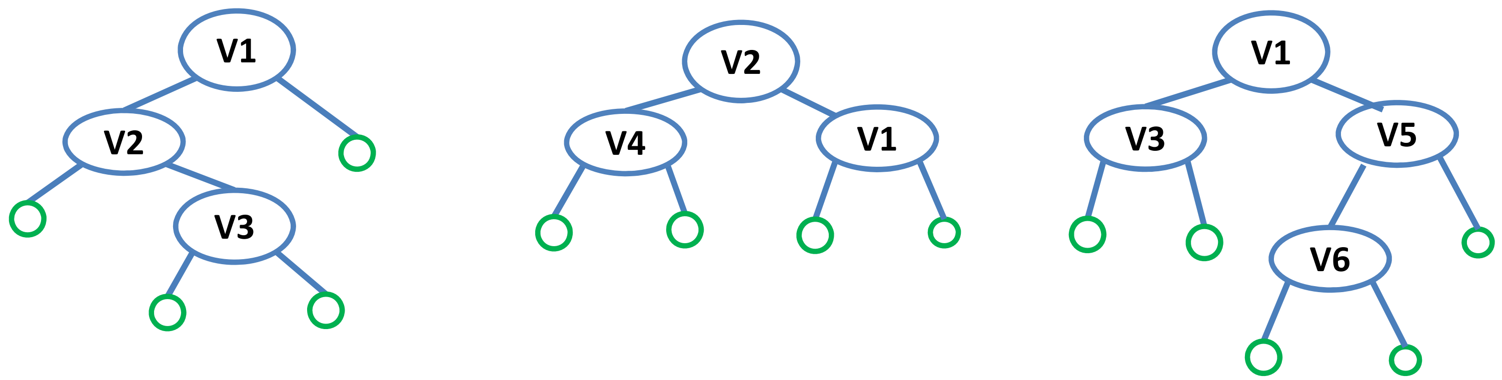


  - If each bootstrap sample takes 67% of the training data, then after building T trees every training example will have been OOB (and hence a valid test example) for about T/3 times.
  - For each training example, take the majority vote of all T/3 test predictions to get the forest's prediction* and compare with the actual class value. Output 1 if forest prediction != actual, else output 0
  - Sum over all training examples to get error estimate for the forest

** For regression problems, average all T/3 test predictions to get the forest prediction. Then compute MSE as $\Sigma_{\text{training examples}}$ (prediction – actual)**2*

Measuring Variable Importance

- For a single tree the order in which the variables occur in the tree is a measure of their relative importance to the prediction



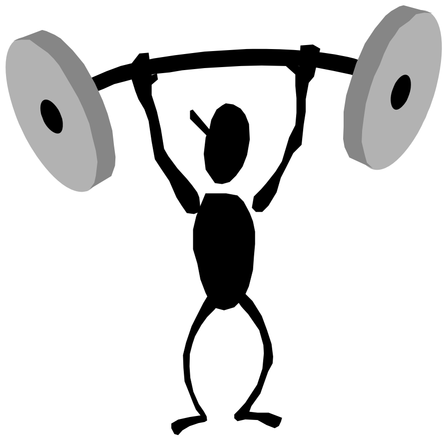
- For a forest?
  - Naïve method: Count the number of times the variable occurs in all of the trees, more occurrences => more important
  - Better method: sum the total reduction in impurity (the decreases in the Gini index) for all nodes that test the variable

Measuring Variable Importance

- Permutation Method
  - Randomly shuffle the values of a given input variable to "break" the bond of the variable to the response. Then the difference of the model accuracy before and after the shuffling is a measure of how important the variable is for predicting the response
- Detailed Method
  1. Test every tree on its own OOB examples. For each training example ***e*** count the votes for the correct class (call this $\text{NormalCorrectVotes}_e$)
  2. For each input variable ***v***:
     - For each tree ***t***:
       - Randomly permute the values for ***v*** in the OOB examples and retest the tree
     - For each training example, count the votes for the correct class
     - $\text{Importance}_v = \text{average}\left[\dfrac{\text{NormalCorrectVotes}_e - \text{ShuffledCorrectVotes}_e}{\text{TotalVotes}_e}\right]$

Boosting

- Can a set of **weak learners** create a single **strong learner**?
  - A theoretical question that triggered much research in 1980's & 1990's
  - A weakly learned model is only slightly better than random guessing
  - A strongly learned model is arbitrarily well-correlated with the truth
- Boosting essentials:
  - Build a model (but don't 100% over-fit the data!)
  - Increase weights of the training examples the model gets wrong
  - Retrain a new model using the weighted training set
  - Repeat many times…



Incorrectly classified examples count for more when the model is retrained

Basic Boosting Algorithm

1. Weight all training samples equally
2. Train model on train set
3. Compute error of model on train set
4. *Increase weights on train cases that the model gets wrong!*
5. Train new model on re-weighted train set
6. Re-compute errors on weighted train set
7. Increase weights more on cases it still gets wrong
8. Repeat until tired (100+ iterations)
9. Final model: *weighted* prediction of each model (aka base models)

Most well-known & successful boosting algorithm is AdaBoost (Adaptive Boosting, *Freund and Schapire, 94*)

Recent popular algorithms: SMOTEboost, Gradient Boosting

AdaBoost* (Adaptive Boosting)

Given: $(x_1, y_1), \ldots, (x_m, y_m)$ where $x_i \in \mathscr{X}$, $y_i \in \{-1, +1\}$. ← The training examples

Initialize: $D_1(i) = 1/m$ for $i = 1, \ldots, m$. ← The training example weights

For $t = 1, \ldots, T$:

- Train weak learner using distribution D_t. ← Train a model (build a classifier)
- Get weak hypothesis $h_t : \mathscr{X} \to \{-1, +1\}$.
- Aim: select h_t with low weighted error:

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

← Goal of classifier is to reduce weighted error relative to Dt

Cases where the prediction does not equal the real class value

- Choose $\alpha_t = \frac{1}{2} \ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$.
- Update, for $i = 1, \ldots, m$:

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

← Re-weight the examples

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

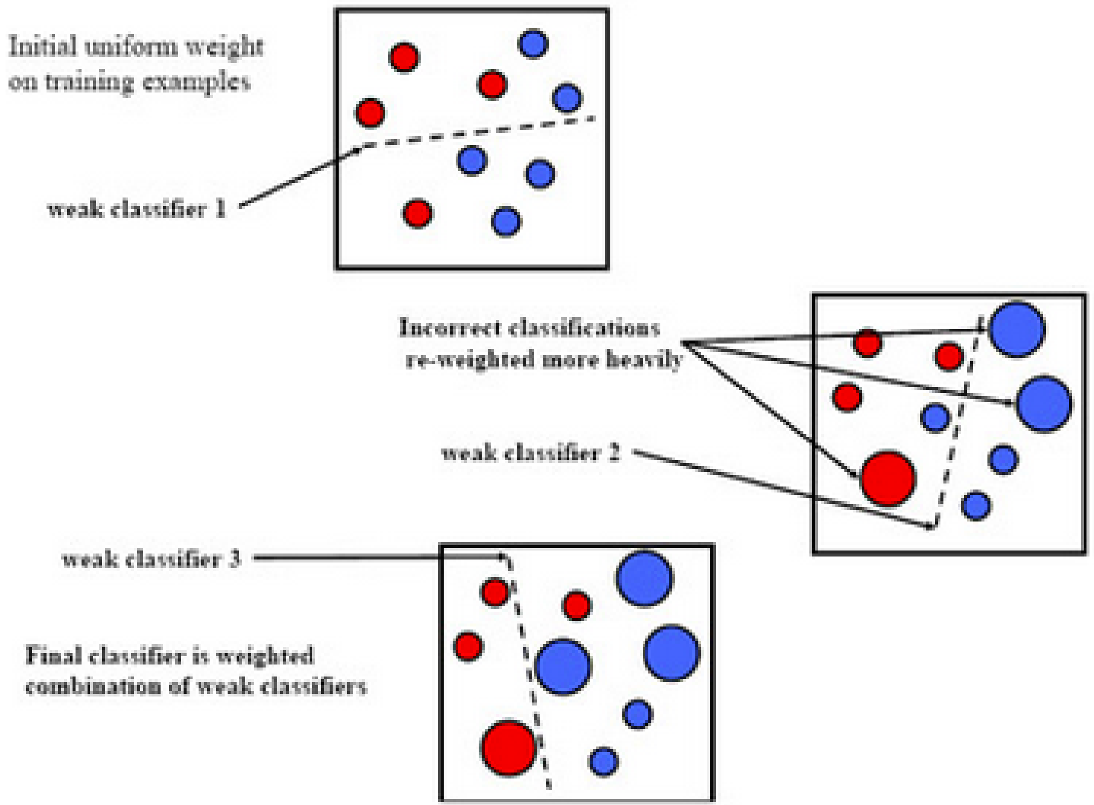
Output the final hypothesis:

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

← The “final” prediction is the weighted average of all of the weak classifiers

**Freund and Schapire, 94*

AdaBoost - Conceptual



$$H(x) = sign(\alpha_1 h_1(x) + \alpha_2 h_2(x) + \alpha_3 h_3(x))$$

Boosting versus Bagging/RF

- In practice bagging/RF almost always helps
- Bagging doesn't work as well with stable models
  - Boosting and RF might still help.
- Often, boosting helps more than bagging
  - Boosting might hurt performance on noisy datasets
  - Bagging/RF don't have this problem.
- Bagging/RF is easier to parallelize

A good background read!

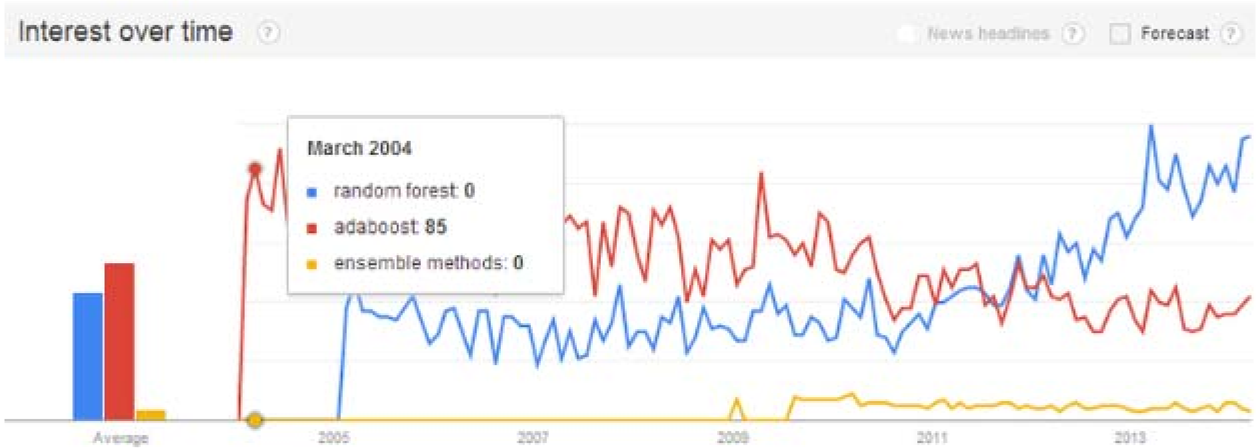
March 25, 2014

A Thumbnail History of Ensemble Methods

By Mike Bowles

Ensemble methods are the backbone of machine learning techniques. However, it can be a daunting subject for someone approaching it for the first time, so we asked Mike Bowles, machine learning expert and serial entrepreneur to provide some context.

Ensemble Methods are among the most powerful and easiest to use of predictive analytics algorithms and R programming language has an outstanding collection that includes the best performers – Random Forest, Gradient Boosting and Bagging as well as big data versions that are available through Revolution Analytics.



See http://blog.revolutionanalytics.com/2014/03/a-thumbnail-history-of-ensemble-methods.html

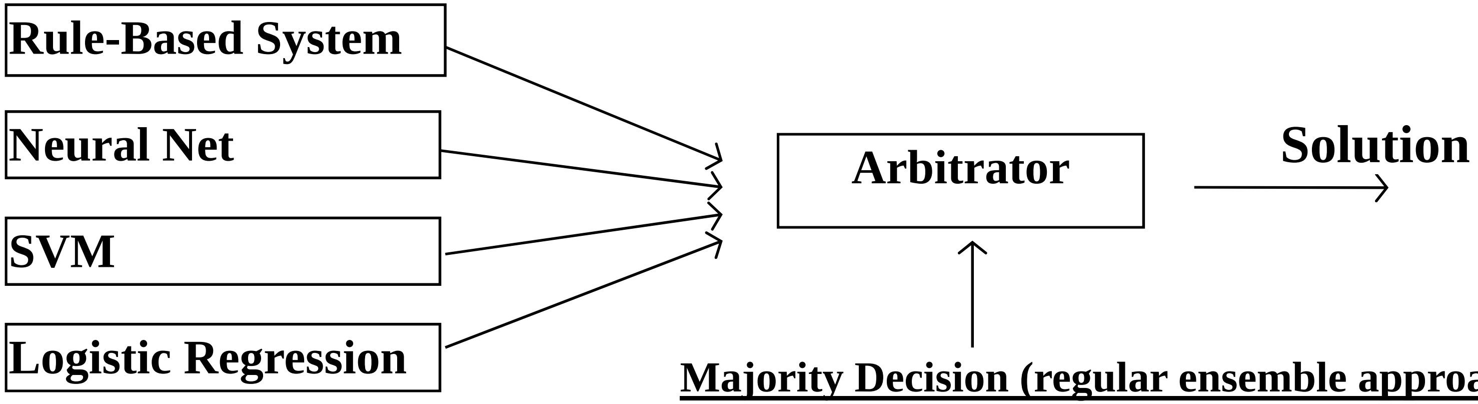
Multiple Classifier Systems (MCS)

- In an Ensemble, the models cooperate to make a prediction
  - Having lots of ensemble members works best

- In “Mixture of Experts” approach, each classifier is expert in certain situations (Jordon, Jacobs, 1994)
  - Each model type has different strengths and weaknesses
  - Usually have relatively small number of experts

Mixture of Experts Example

- Different solution strategies (experts) offer alternative solutions. Another process decides which solution to accept or how to combine the solutions, e.g. majority vote algorithm.
- This architecture is also known as stacking*



Individual Experts

Majority Decision (regular ensemble approach)
If majority agree then good decision, else unreliable decision

OR…

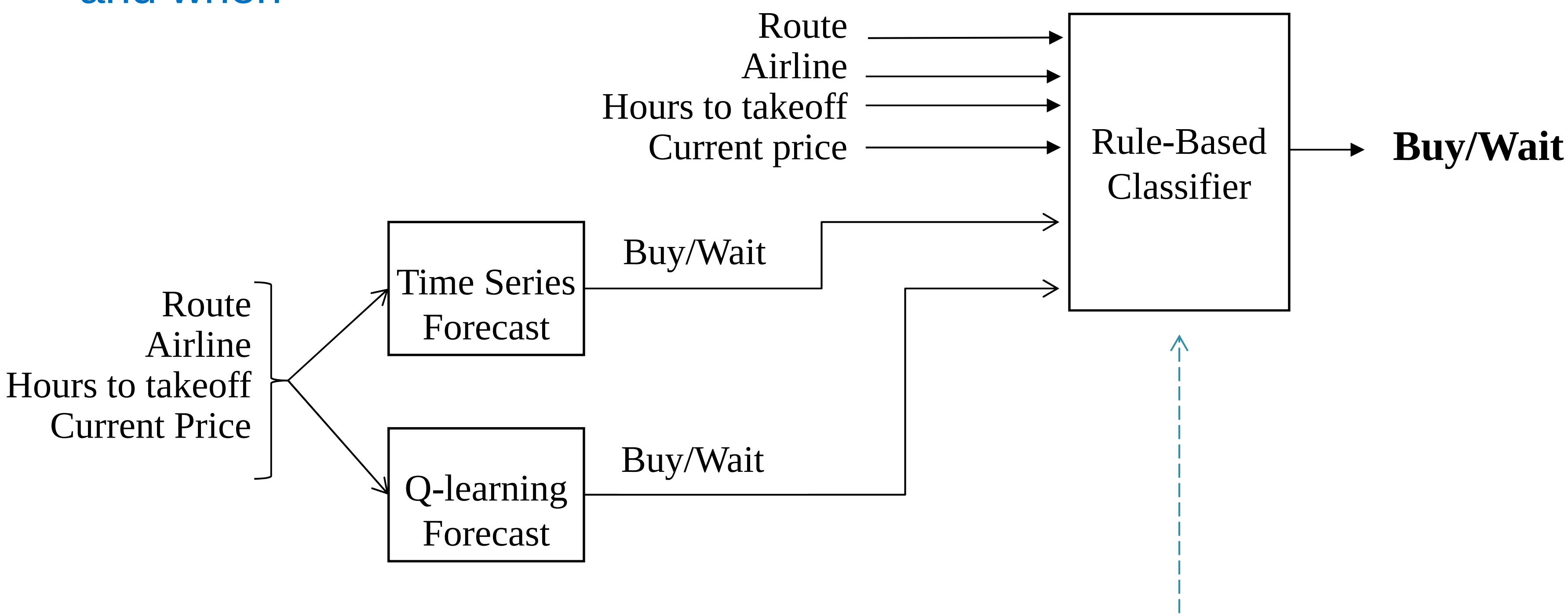
Weighted Decision
Weight expert judgements according to circumstances

Best Expert Only
Decide which expert is most appropriate for current situation

**Stacking (sometimes called stacked generalization) involves training a learning algorithm to combine the predictions of several other learning algorithms (Wikipedia)*

Mixture of Experts Example

- Airfare Price prediction
- The Experts have same skills (Buy/Wait decision) but sometimes one is better than the other! The arbitrator helps decide which to use and when

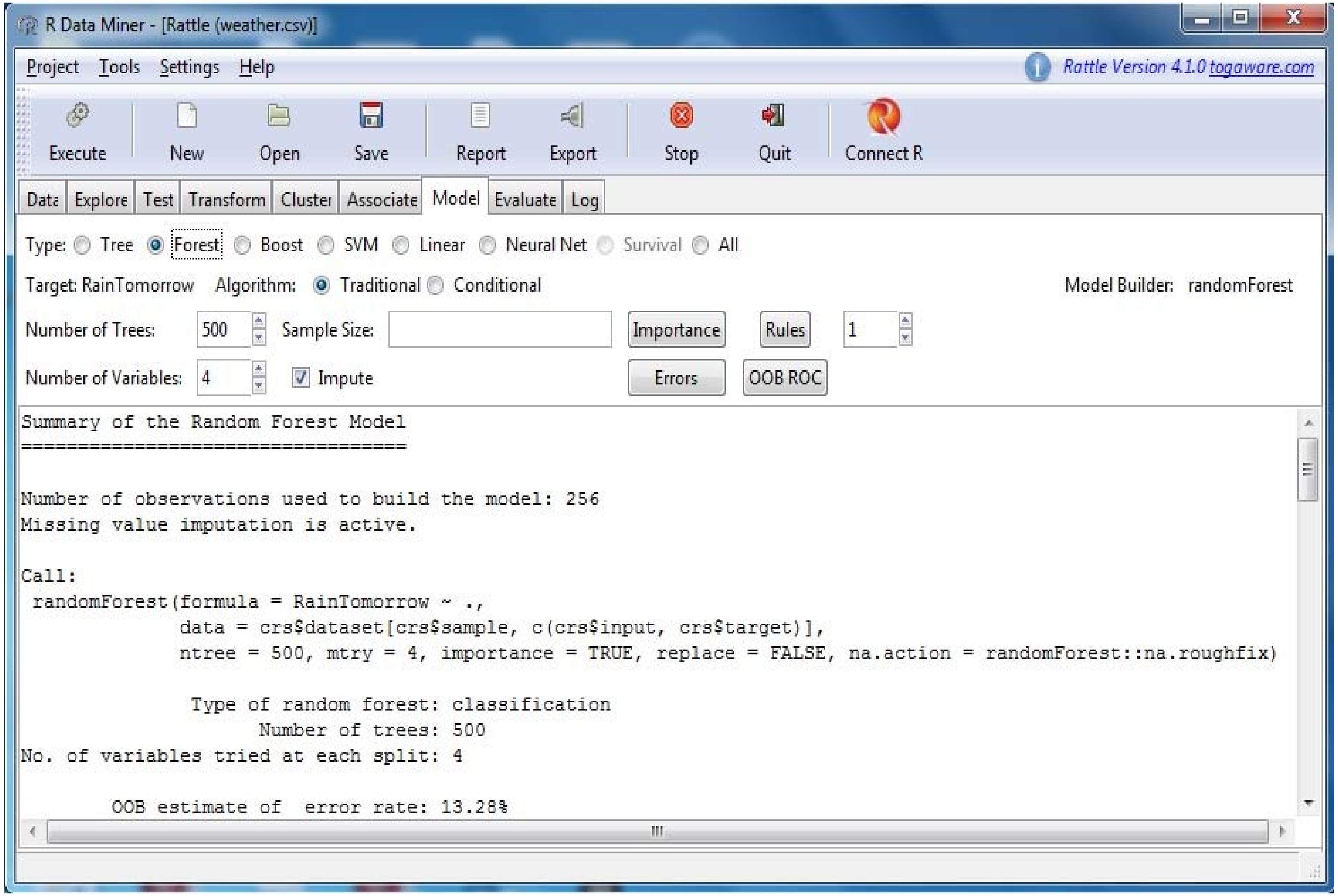


IF hours-before-takeoff $>= 480$ AND $airline = United$ AND $price >= 360$ AND $TS = buy$ AND $QL = wait$ THEN $wait$

Ensembles Summary

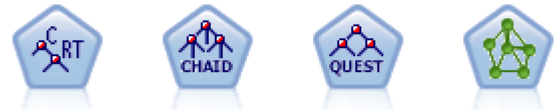
- Ensembles
  - Using multiple models to reduce variance and increase accuracy
  - Usually work by averaging across models
  - Works best if models don’t agree with each other (need model variance)
  - Usually refers to multiple models of same type
  - Bagging & Boosting are the most popular generic methods
  - Random Forest increasingly popular
- Multiple Classifier Systems
  - Combining a smaller number of different model types
  - Can also be thought of as Ensembles (by SPSS Modeler)
  - Allows for other model combination methods apart from averaging

Bagging & Boosting in R & Rattle

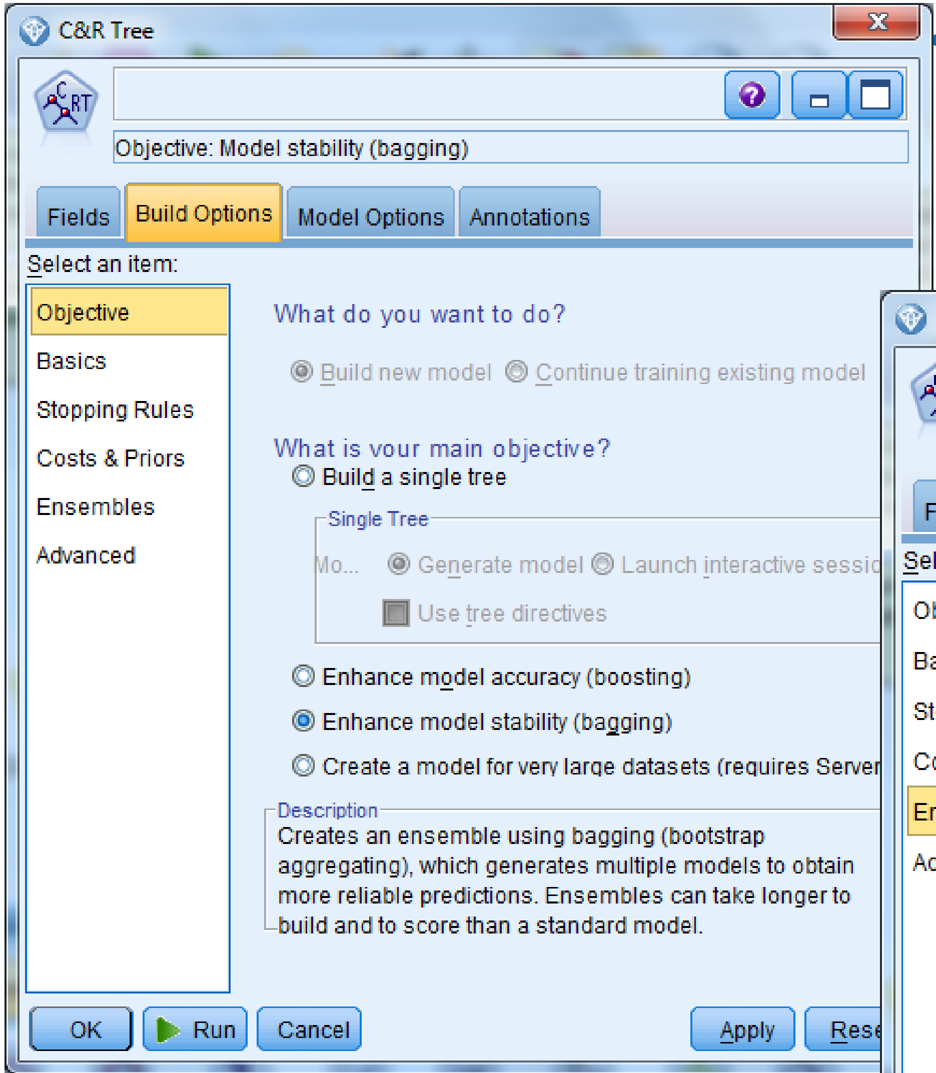


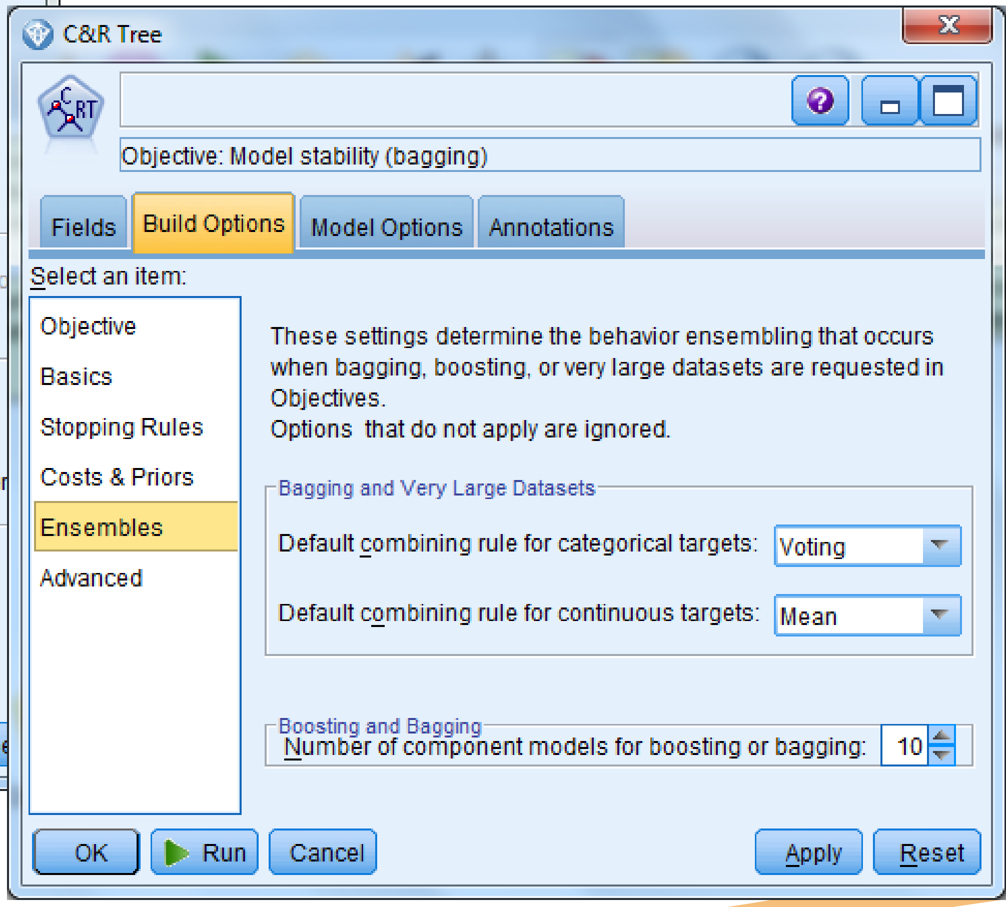
Bagging & Boosting in SPSS Modeler

- Some model nodes implement bagging & boosting

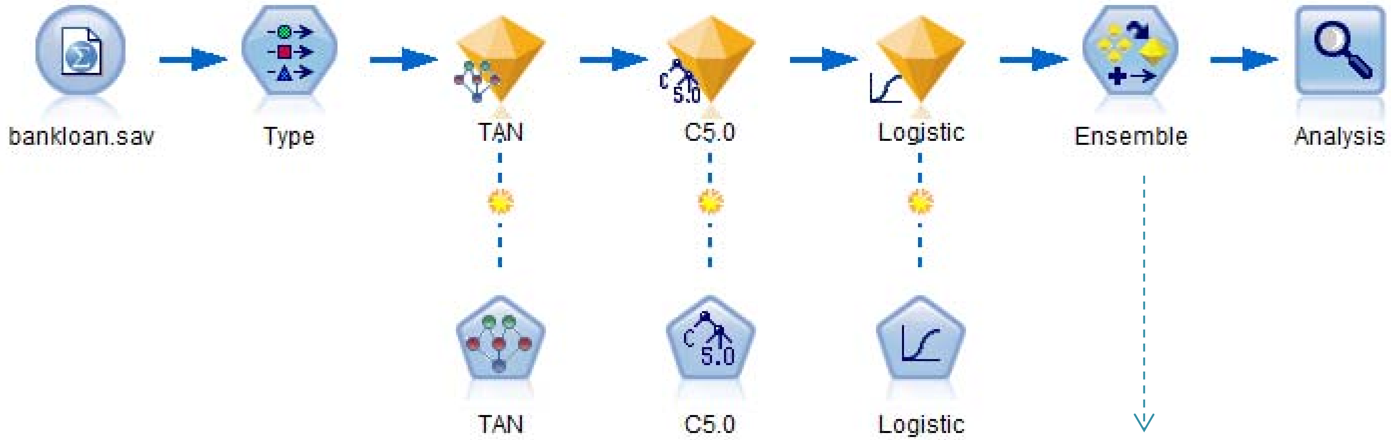


C&R Tree CHAID Quest Neural Net





Building Ensembles in SPSS Modeler



Ensemble method	Field name
Voting Confidence-weighted voting Raw-propensity-weighted voting Raw-propensity-weighted voting Highest confidence wins	*$XFC_<field>*
Average raw propensity	*$XFRP_<field>*
Average adjusted raw propensity	*$XFAP_<field>*