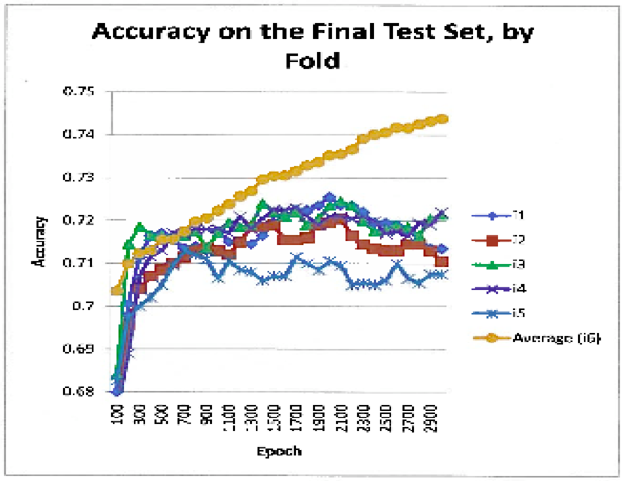


Bias/Variance Tradeoff

Model Loss (Error)

- Squared loss of model on test case i:

$$\left(Learn(x_i, D) - Truth(x_i)\right)^2$$

- Expected prediction error:

$$\left\langle \left(Learn(x, D) - Truth(x)\right)^2 \right\rangle_D$$

Bias/Variance Decomposition

$$\left\langle \left(L(x,D) - T(x)\right)^2 \right\rangle_D = Noise^2 + Bias^2 + Variance$$

$Noise^2$ = lower bound on performance

$Bias^2$ = (expected error due to model mismatch)^2

$Variance$ = variation due to train sample and randomization

$Bias^2$

- Low bias
  - linear regression applied to linear data
  - 2nd degree polynomial applied to quadratic data
  - ANN with many hidden units trained to completion
- High bias
  - constant function
  - linear regression applied to non-linear data
  - ANN with few hidden units applied to non-linear data

Variance

- Low variance
  - constant function
  - model independent of training data
  - model depends on stable measures of data
    - mean
    - median
- High variance
  - high degree polynomial
  - ANN with many hidden units trained to completion

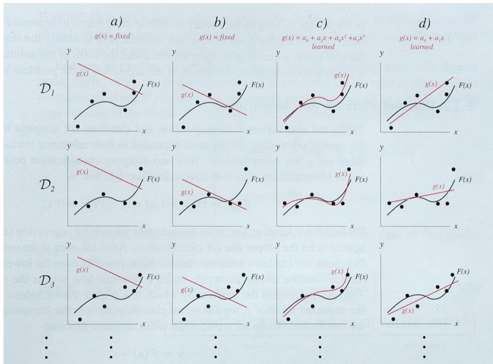
Sources of Variance in Supervised Learning

- noise in targets or input attributes
- bias (model mismatch)
- training sample
- randomness in learning algorithm
  - neural net weight initialization
- randomized subsetting of train set:
  - cross validation, train and early stopping set

Bias/Variance Tradeoff

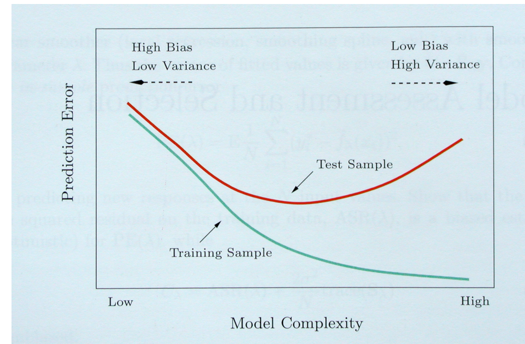
- ($bias^2$+variance) is what counts for prediction
- Often:
  - low bias => high variance
  - low variance => high bias
- Tradeoff:
  - $bias^2$ vs. variance

Bias/Variance Tradeoff



Duda, Hart, Stork "Pattern Classification", 2nd edition, 2001

Bias/Variance Tradeoff



Hastie, Tibshirani, Friedman "Elements of Statistical Learning" 2001

Reduce Variance Without Increasing Bias

- Averaging reduces variance:

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

- Average models to reduce model variance
- One problem:
  - only one train set
  - where do multiple models come from?

Bagging: Bootstrap Aggregation

- Leo Breiman (1994)
- Bootstrap Sample:
  - draw sample of size |D| with replacement from D

$$\text{Train } L_i\big(BootstrapSample_i(D)\big)$$

$$\text{Regression}: L_{bagging} = \overline{L_i}$$

$$\text{Classification}: L_{bagging} = Plurality\big(L_i\big)$$

Bagging

- Best case:

$$Var(Bagging(L(x,D))) = \frac{Variance(L(x,D))}{N}$$

- In practice:
  - models are correlated, so reduction is smaller than 1/N
  - variance of models trained on fewer training cases usually somewhat larger
  - stable learning methods have low variance to begin with, so bagging may not help much

Bagging Results

Table 1 Missclassification Rates (Percent)

Data Set	$\bar{e}_S$	$\bar{e}_B$	**Decrease**
waveform	29.0	19.4	33%
heart	10.0	5.3	47%
breast cancer	6.0	4.2	30%
ionosphere	11.2	8.6	23%
diabetes	23.4	18.8	20%
glass	32.0	24.9	22%
soybean	14.5	10.6	27%

Breiman "Bagging Predictors" Berkeley Statistics Department TR#421, 1994

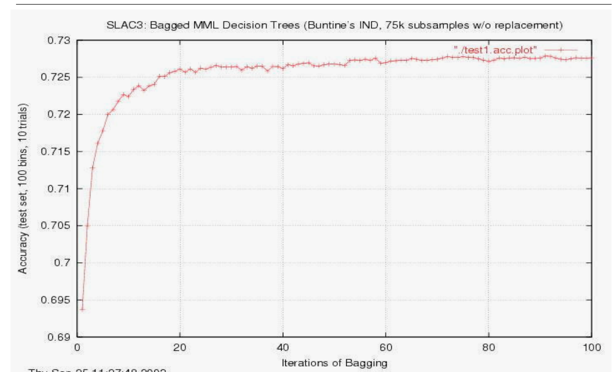
How Many Bootstrap Samples?

Table 5.1
Bagged Missclassification Rates (%)

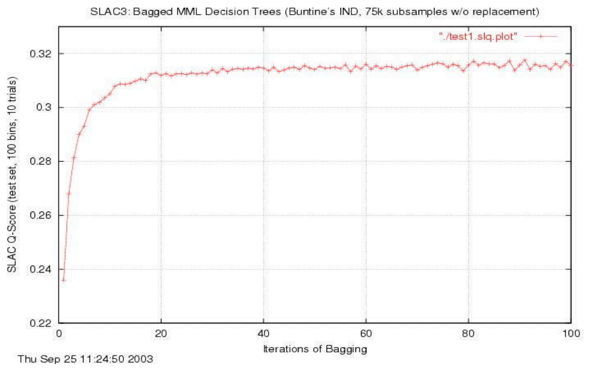
No. Bootstrap Replicates	Missclassification Rate
10	21.8
25	19.5
50	19.4
100	19.4

Breiman "Bagging Predictors" Berkeley Statistics Department TR#421, 1994

More bagging results



More bagging results



Bagging with cross validation

- Train neural networks using 4-fold CV
  - Train on 3 folds earlystop on the fourth
  - At the end you have 4 neural nets

- How to make predictions on new examples?

Bagging with cross validation

- Train neural networks using 4-fold CV
  - Train on 3 folds earlystop on the fourth
  - At the end you have 4 neural nets

- How to make predictions on new examples?
  - Train a neural network until the mean earlystopping point
  - Average the predictions from the four neural networks

Can Bagging Hurt?

Can Bagging Hurt?

- Each base classifier is trained on less data
  - Only about 63.2% of the data points are in any bootstrap sample
- However the final model has seen all the data
  - On average a point will be in >50% of the bootstrap samples

Reduce Bias^2 and Decrease Variance?

- Bagging reduces variance by averaging
- Bagging has little effect on bias
- Can we average *and* reduce bias?
- Yes:

Boosting

Boosting

- Freund & Schapire:
  - theory for "weak learners" in late 80's
- Weak Learner: performance on ***any*** train set is slightly better than chance prediction
- intended to answer a theoretical question, not as a practical way to improve learning
- tested in mid 90's using not-so-weak learners
- works anyway!

Boosting

- Weight all training samples equally
- Train model on train set
- Compute error of model on train set
- *Increase weights on train cases model gets wrong!*
- Train new model on re-weighted train set
- Re-compute errors on weighted train set
- Increase weights again on cases model gets wrong
- Repeat until tired (100+ iterations)
- Final model: *weighted* prediction of each model

Boosting

Initialization →

Algorithm AdaBoost.M1
Input: sequence of m examples $\langle (x_1, y_1), \ldots, (x_m, y_m) \rangle$
with labels $y_i \in Y = \{1, \ldots, k\}$
weak learning algorithm **WeakLearn**
integer T specifying number of iterations

Initialize $D_1(i) = 1/m$ for all i.

Iteration →

Do for $t = 1, 2, \ldots, T$:

1. Call **WeakLearn**, providing it with the distribution D_t.
2. Get back a hypothesis $h_t : X \to Y$.
3. Calculate the error of h_t: $\epsilon_t = \sum_{i: h_t(x_i) \neq y_i} D_t(i)$.
   If $\epsilon_t > 1/2$, then set $T = t - 1$ and abort loop.
4. Set $\beta_t = \epsilon_t / (1 - \epsilon_t)$.
5. Update distribution D_t:
   $$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \times \begin{cases} \beta_t & \text{if } h_t(x_i) = y_i \\ 1 & \text{otherwise} \end{cases}$$
   where Z_t is a normalization constant (chosen so that D_{t+1} will be a distribution).

Final Model →

Output the final hypothesis:
$$h_{fin}(x) = \arg\max_{y \in Y} \sum_{t: h_t(x) = y} \log \frac{1}{\beta_t}.$$

Boosting: Initialization

Algorithm AdaBoost.M1
Input: sequence of m examples $\langle (x_1, y_1), \ldots, (x_m, y_m) \rangle$
with labels $y_i \in Y = \{1, \ldots, k\}$
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Boosting: Iteration

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

Boosting: Prediction

Output the final hypothesis:
$$h_{fin}(x) = \arg\max_{y \in Y} \sum_{t: h_t(x) = y} \log \frac{1}{\beta_t}.$$

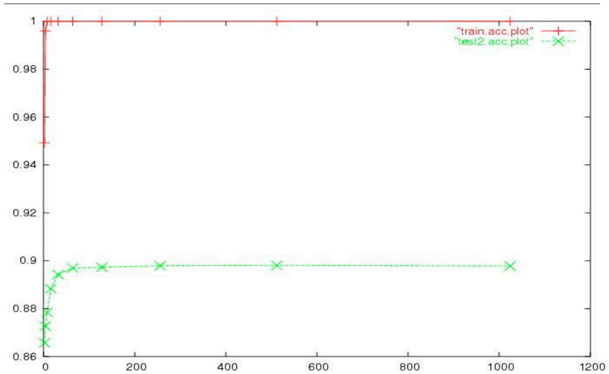
Weight updates

- Weights for incorrect instances are multiplied by 1/(2Error_i)
  - Small train set errors cause weights to grow by several orders of magnitude
- Total weight of misclassified examples is 0.5
- Total weight of correctly classified examples is 0.5

Reweighting vs Resampling

- Example weights might be harder to deal with
  - Some learning methods can't use weights on examples
  - Many common packages don't support weighs on the train
- We can resample instead:
  - Draw a bootstrap sample from the data with the probability of drawing each example is proportional to it's weight
- Reweighting usually works better but resampling is easier to implement

Boosting Performance



Boosting vs. Bagging

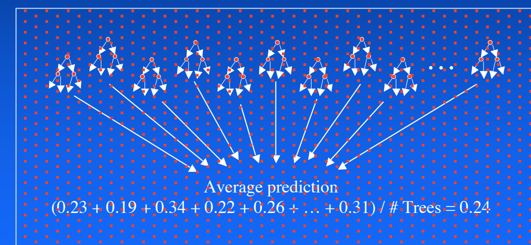
- Bagging doesn't work so well with stable models. Boosting might still help.
- Boosting might hurt performance on noisy datasets. Bagging doesn't have this problem
- In practice bagging almost always helps.

Boosting vs. Bagging

- On average, boosting helps more than bagging, but it is also more common for boosting to hurt performance.
- The weights grow exponentially. Code must be written carefully (store log of weights, …)
- Bagging is easier to parallelize.

Bagged Decision Trees

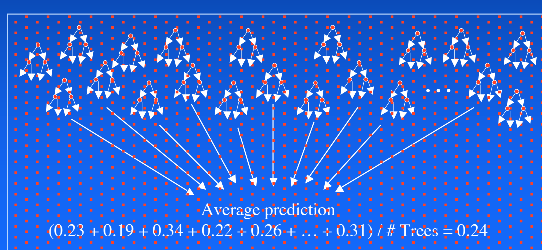
- Draw 100 bootstrap samples of data
- Train trees on each sample -> 100 trees
- Un-weighted average prediction of trees



- Marriage made in heaven. Highly under-rated!

Random Forests (Bagged Trees++)

- Draw ***1000+*** bootstrap samples of data
- ***Draw sample of available attributes at each split***
- Train trees on each sample/attribute set -> ***1000+*** trees
- Un-weighted average prediction of trees



Model Averaging

- Almost always helps
- Often easy to do
- Models shouldn’t be too similar
- Models should all have pretty good performance (not too many lemons)
- When averaging, favor low bias, high variance
- Models can individually overfit
- Not just in ML

Out of Bag Samples

- With bagging, each model trained on about 63% of training sample
- That means each model does not use 37% of data
- Treat these as test points!
  - Backfitting in trees
  - Pseudo cross validation
  - Early stopping sets