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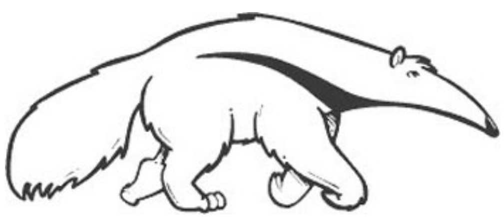
Machine Learning and Data Mining

Ensembles of Learners

Prof. Alexander Ihler

Fall 2012



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Ensemble methods

- Why learn one classifier when you can learn many?
- Ensemble: combine many predictors
  - (Weighted) combinations of predictors
  - May be same type of learner or different

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"Who wants to be a millionaire?"

Ensemble methods

- Why learn one classifier when you can learn many?
- Ensemble: combine many predictors
  - (Weighted) combinations of predictors
  - May be same type of learner or different

Various options for getting help:

"Who wants to be a millionaire?"

Simple ensembles

- “Committees”
  - Unweighted average / majority vote

Simple ensembles

- "Committees"
  - Unweighted average / majority vote

- Weighted averages
  - Up-weight "better" predictors
  - Ex: Classes: +1 , -1 , weights alpha:

$\hat{y}_1 = f_1(x_1, x_2, \ldots)$

$\hat{y}_2 = f_2(x_1, x_2, \ldots)$ => $\hat{y}_e = \text{sign}(\sum \alpha_i \hat{y}_i)$

…

Simple ensembles

- One option: train a "predictor of predictors"
  - Treat individual predictors as features

    $\hat{y}_1 = f_1(x_1, x_2, \ldots)$

    $\hat{y}_2 = f_2(x_1, x_2, \ldots)$ => $\hat{y}_e = f_e(\hat{y}_1, \hat{y}_2, \ldots)$

    …

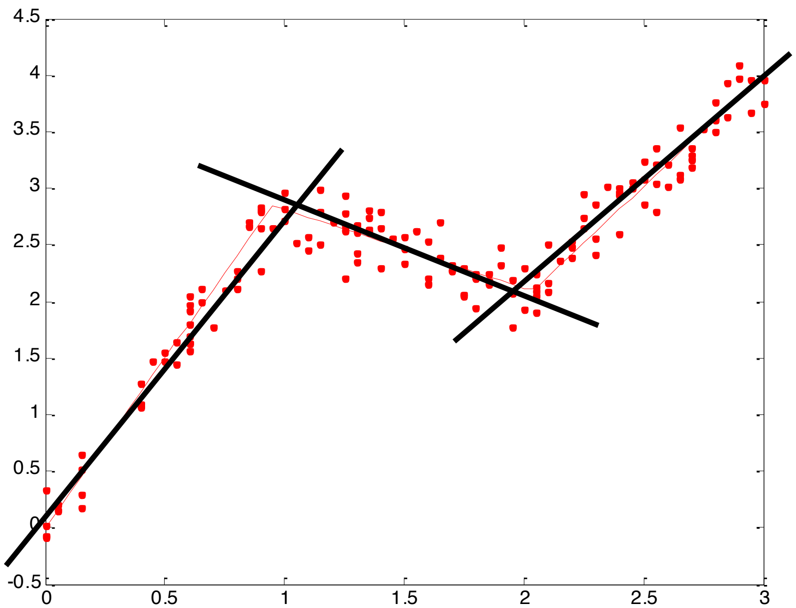
  - Similar to multi-layer perceptron idea

  - Special case: binary, f_e linear => weighted vote

  - Can train ensemble weights f_e on validation data

Mixtures of experts

- Can make weights depend on x
  - Weight $\alpha_i(x)$ indicates “expertise”
  - Combine: weighted avg or just pick largest



Mixture of three linear predictor experts

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Ensembles: Bagging

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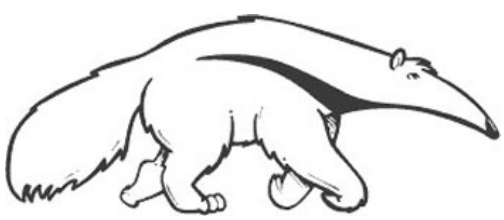

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Ensemble methods

- Why learn one classifier when you can learn many?
  - "Committee": learn K classifiers, average their predictions
- "Bagging" = bootstrap aggregation
  - Learn many classifiers, each with only part of the data
  - Combine through model averaging
- Remember overfitting: "memorize" the data
  - Used test data to see if we had gone too far
  - Cross-validation
    - Make many splits of the data for train & test
    - Each of these defines a classifier
    - Typically, we use these to check for overfitting
    - Could we instead combine them to produce a better classifier?

Bagging

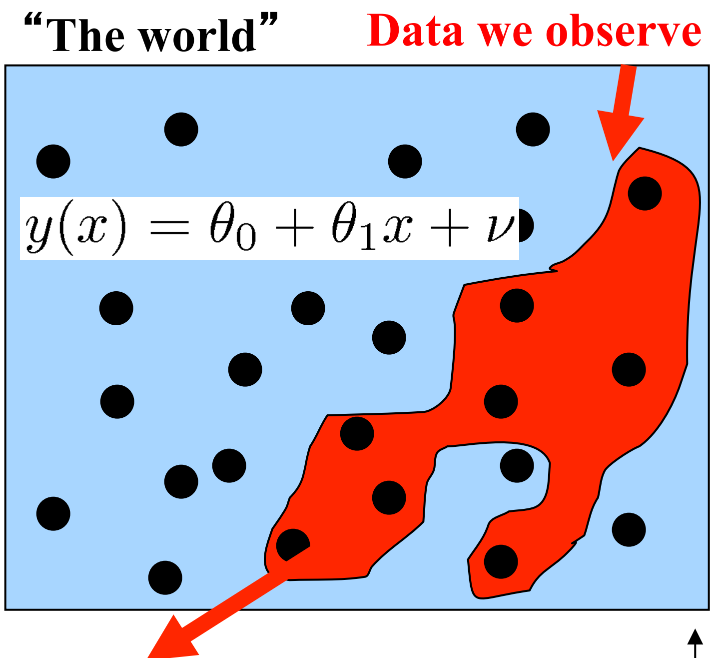
- Bootstrap
  - Create a random subset of data by sampling
  - Draw N' of the N samples with replacement (sometimes w/o)

- Bagging
  - Repeat K times
    - Create a training set of N' < N examples
    - Train a classifier on the random training set
  - To test, run each trained classifier
    - Each classifier votes on the output, take majority
    - For regression: each regressor predicts, take average

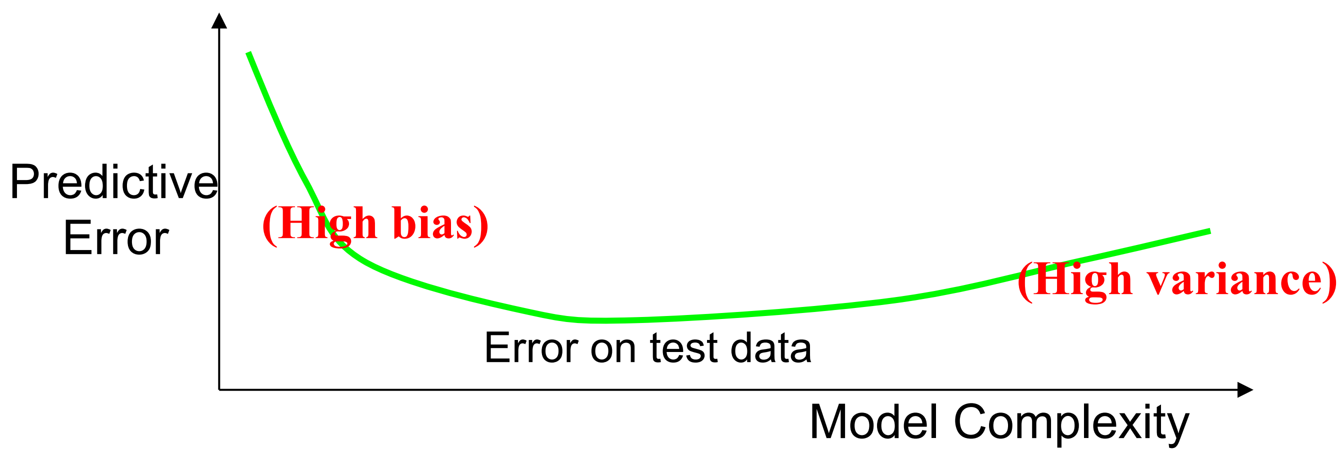
- Notes:
  - Some complexity control: harder for each to memorize data
    - Doesn't work for linear models (e.g. linear regression)
    - Perceptrons OK (linear + threshold = nonlinear)

Bias / Variance

- We only see a little bit of data
- Can decompose error into two parts
  - Bias – error due to model choice
    - Can our model represent the true best predictor?
    - Gets better with more complexity
  - Variance – randomness due to data size
    - Better w/ more data, worse w/ complexity

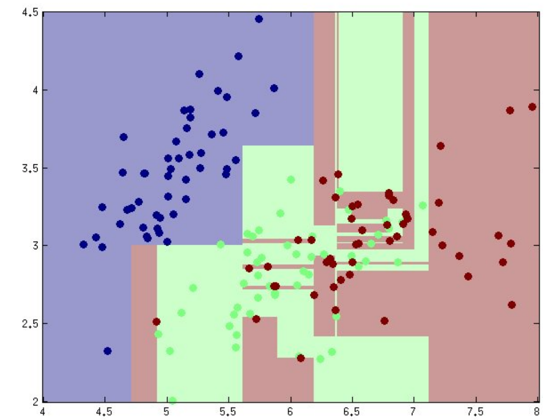


$$\hat{y}(x) = \hat{\theta}_0 + \hat{\theta}_1 x$$



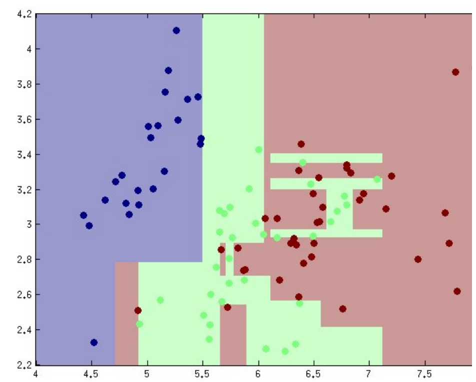
Bagged decision trees

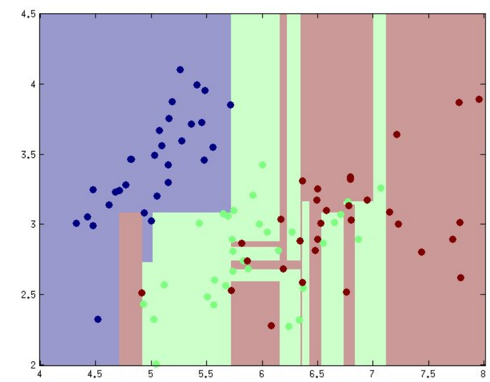
- Randomly resample data
- Learn a decision tree for each

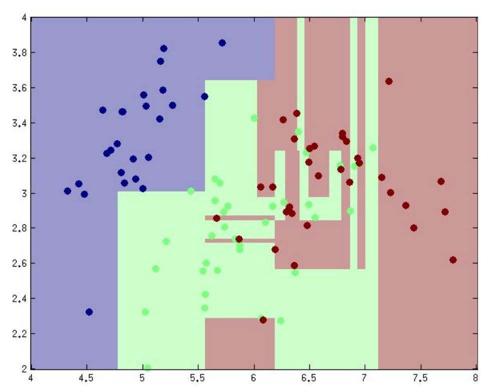


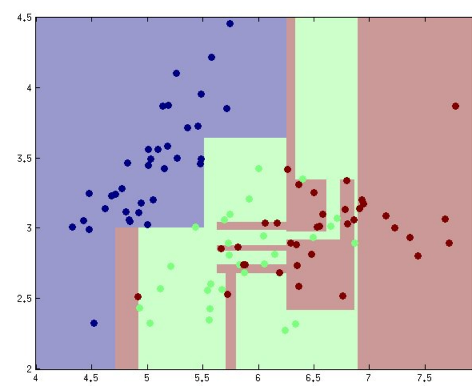
Full data set

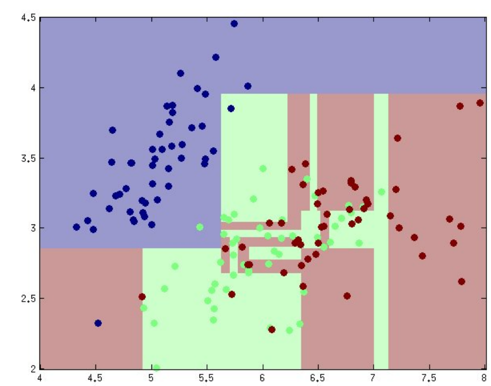
Simulates "equally likely" data sets we could have observed instead, & their classifiers





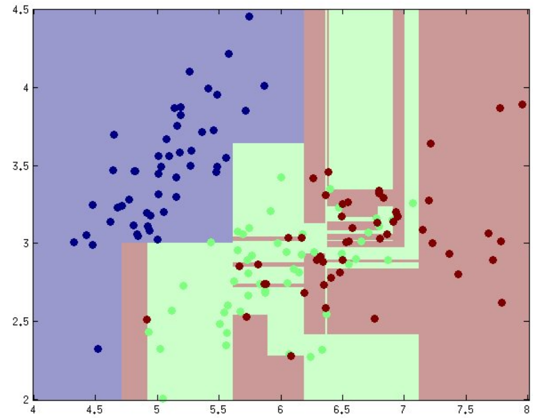






Bagged decision trees

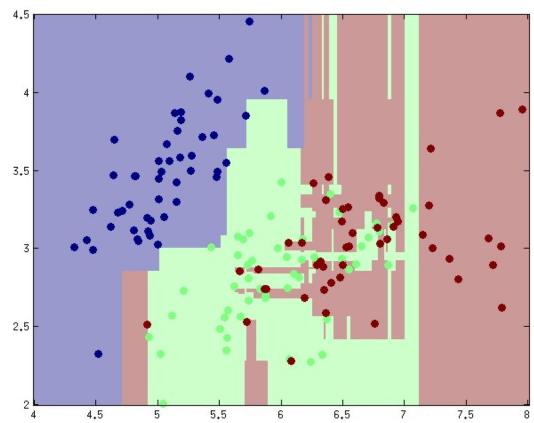
- Average over collection
  - Classification: majority vote



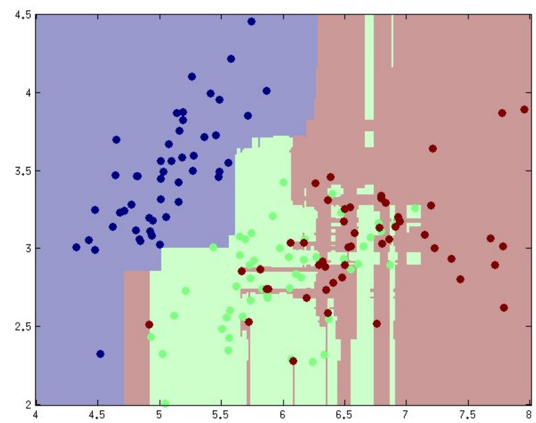
Full data set

- Reduces memorization effect
  - Not every predictor sees each data point
  - Lowers “complexity” of the overall average
  - Usually, better generalization performance

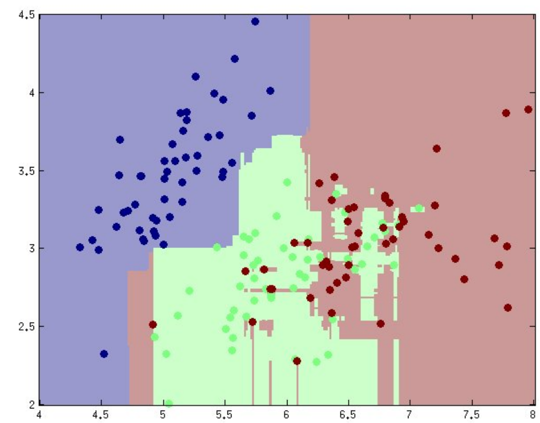
Avg of 5 trees



Avg of 25 trees



Avg of 100 trees



Bagging in Matlab

```
% Data set  X, Y
[N,D] = size(X);
Classifiers = cell(1,Nbag);         % Allocate space
for i=1:Nbag
  ind = ceil( N*rand(Nuse, 1) );    % Bootstrap sample data
  Xi = X(ind, :); Yi = Y(ind, :);   % Select those indices
  Classifiers{i} = Train_Classifier(Xi, Yi);   % Train
end;

% Test data Xtest
[Ntest,D] = size(Xtest);
predict = zeros(Ntest,Nbag);        % Allocate space
for i=1:Nbag,                       % Apply each classifier
  predict(:,i)=Apply_Classifier( Xtest, Classifiers{i});
end;
predict = (mean(predict,2) > 1.5); % Vote on output (1 vs 2)
```

Random forests

- Bagging applied to decision trees
- Problem
  - With lots of data, we usually learn the same classifier
  - Averaging over these doesn't help!
- Introduce extra variation in learner
  - At each step of training, only allow a subset of features
  - Enforces diversity ("best" feature not available)
  - Average over these learners (majority vote)

```
In decisionTreeSplitData2(X,Y):
  For each of a subset of features
    For each possible split
      Score the split  (e.g. information gain)
  Pick the feature & split with the best score
  Recurse on each subset
```

Summary

- Ensembles: collections of predictors
  - Combine predictions to improve performance

- Bagging
  - "Bootstrap aggregation"
  - *Reduces* complexity of a model class prone to overfit
  - In practice
    - Resample the data many times
    - For each, generate a predictor on that resampling
  - Plays on bias / variance trade off
  - Price: more computation per prediction

Machine Learning and Data Mining

Ensembles: Gradient Boosting

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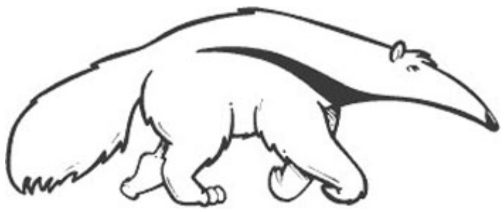

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Ensembles

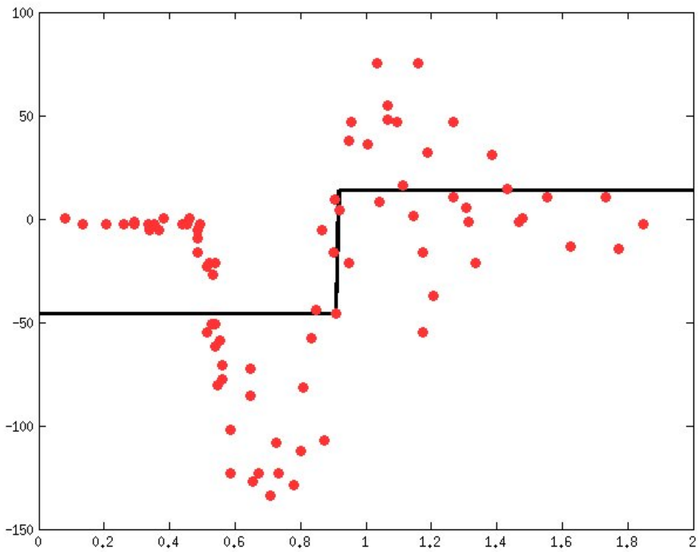
- Weighted combinations of predictors
- “Committee” decisions
  - Trivial example
  - Equal weights (majority vote / unweighted average)
  - Might want to weight unevenly – up-weight better predictors

- Boosting
  - Focus new learners on examples that others get wrong
  - Train learners sequentially
  - Errors of early predictions indicate the “hard” examples
  - Focus later predictions on getting these examples right
  - Combine the whole set in the end
  - Convert many “weak” learners into a complex predictor

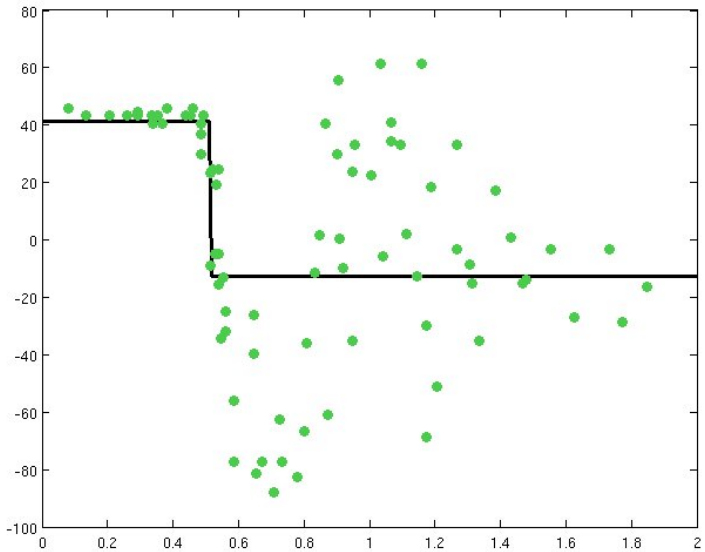
Gradient Boosting

- Learn a regression predictor
- Compute the error residual
- Learn to predict the residual

Learn a simple predictor…



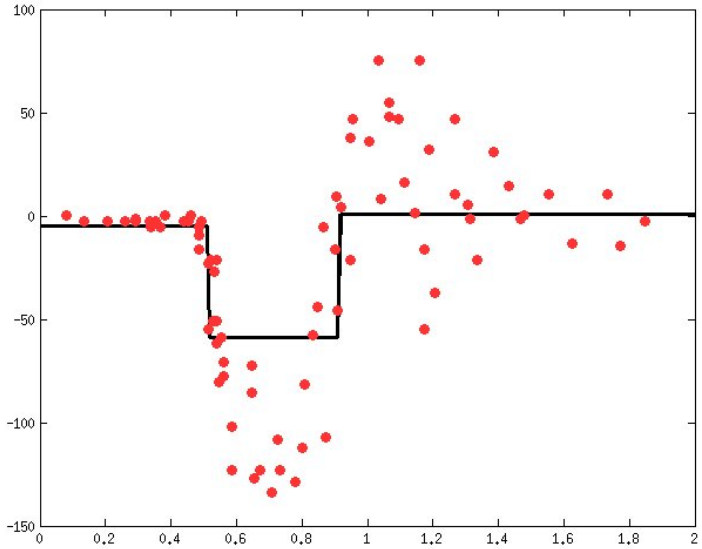
Then try to correct its errors



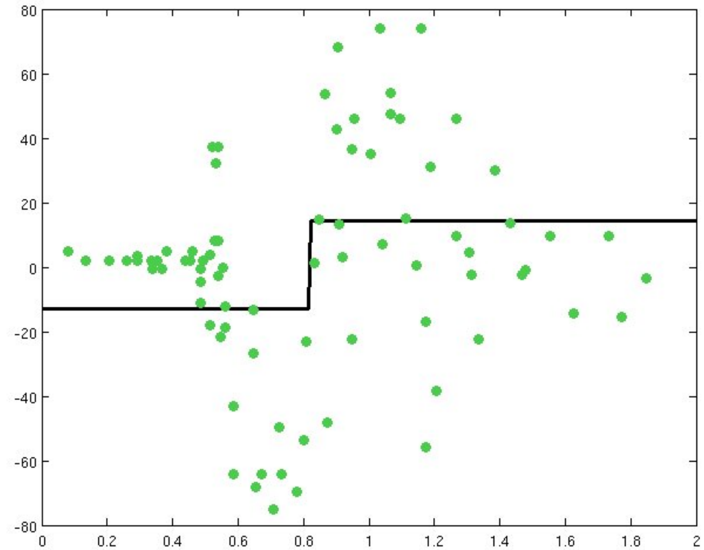
Gradient Boosting

- Learn a regression predictor
- Compute the error residual
- Learn to predict the residual

Combining gives a better predictor…

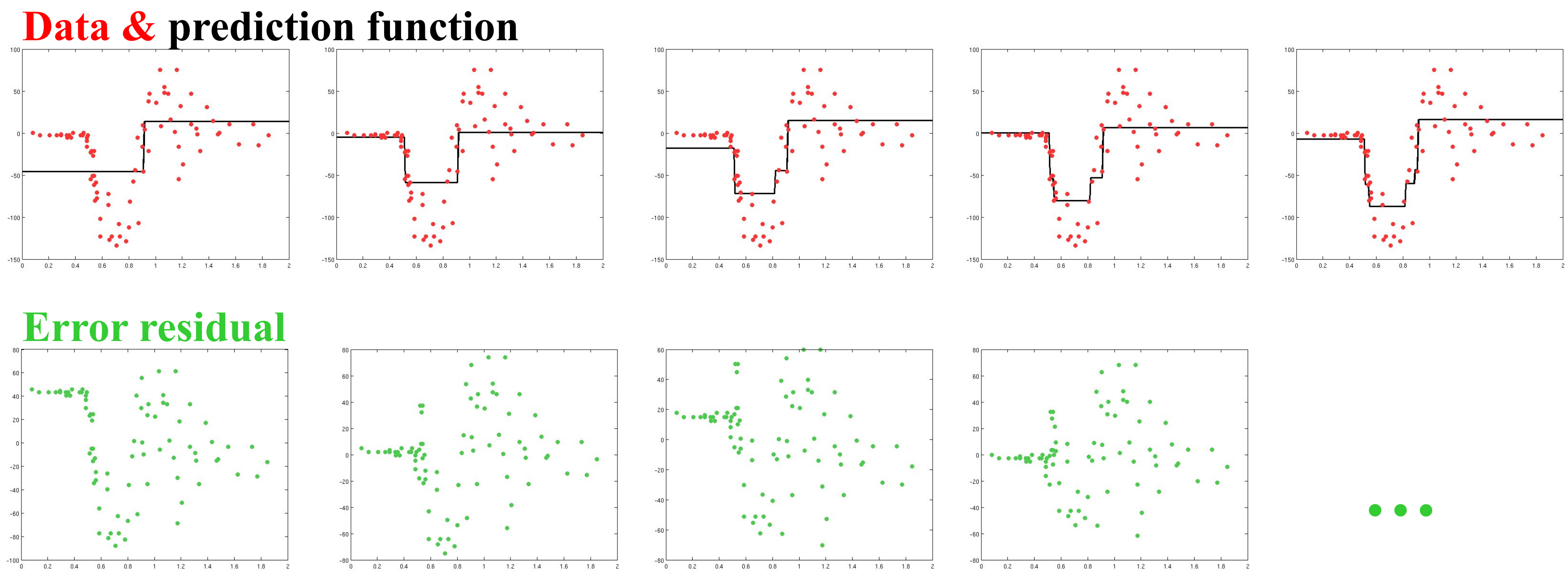


Can try to correct its errors also, & repeat



Gradient Boosting

- Learn sequence of predictors
- Sum of predictions is increasingly accurate
- Predictive function is increasingly complex



Gradient boosting

- Make a set of predictions $\hat{y}[i]$
- The "error" in our predictions is $J(y,\hat{y})$
  - For MSE: $J(.) = \sum (y[i] - \hat{y}[i])^2$
- We can "adjust" $\hat{y}$ to try to reduce the error
  - $\hat{y}[i] = \hat{y}[i] + \text{alpha } f[i]$
  - $f[i] \approx \nabla J(y, \hat{y})$ $= (y[i]-\hat{y}[i])$ for MSE
- Each learner is estimating the gradient of the loss f'n
- Gradient descent: take sequence of steps to reduce J
  - Sum of predictors, weighted by step size alpha

Gradient boosting in Matlab

```
% Data set  X, Y
mu = mean(Y);     % Often start with constant "mean" predictor
dY = Y - mu;      %   subtract this prediction away
For k=1:Nboost,
  Learner{k} = Train_Regressor(X,dY);
  alpha(k) = 1;  % alpha: a "learning rate" or "step size"
  % smaller alphas need to use more classifiers, but tend to
  %   predict better given enough of them

  % compute the residual given our new prediction
  dY = dY - alpha(k) * predict(Learner{k}, X)
end;


% Test data Xtest
[Ntest,D] = size(Xtest);
predict = zeros(Ntest,1);        % Allocate space
For k=1:Nboost,                  % Predict with each learner
  predict = predict + alpha(k)*predict(Learner{k}, Xtest);
end;
```

Summary

- Ensemble methods
  - Combine multiple classifiers to make “better” one
  - Committees, average predictions
  - Can use weighted combinations
  - Can use same or different classifiers

- Gradient Boosting
  - Use a simple regression model to start
  - Subsequent models predict the error residual of the previous predictions
  - Overall prediction given by a weighted sum of the collection

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Ensembles: Boosting

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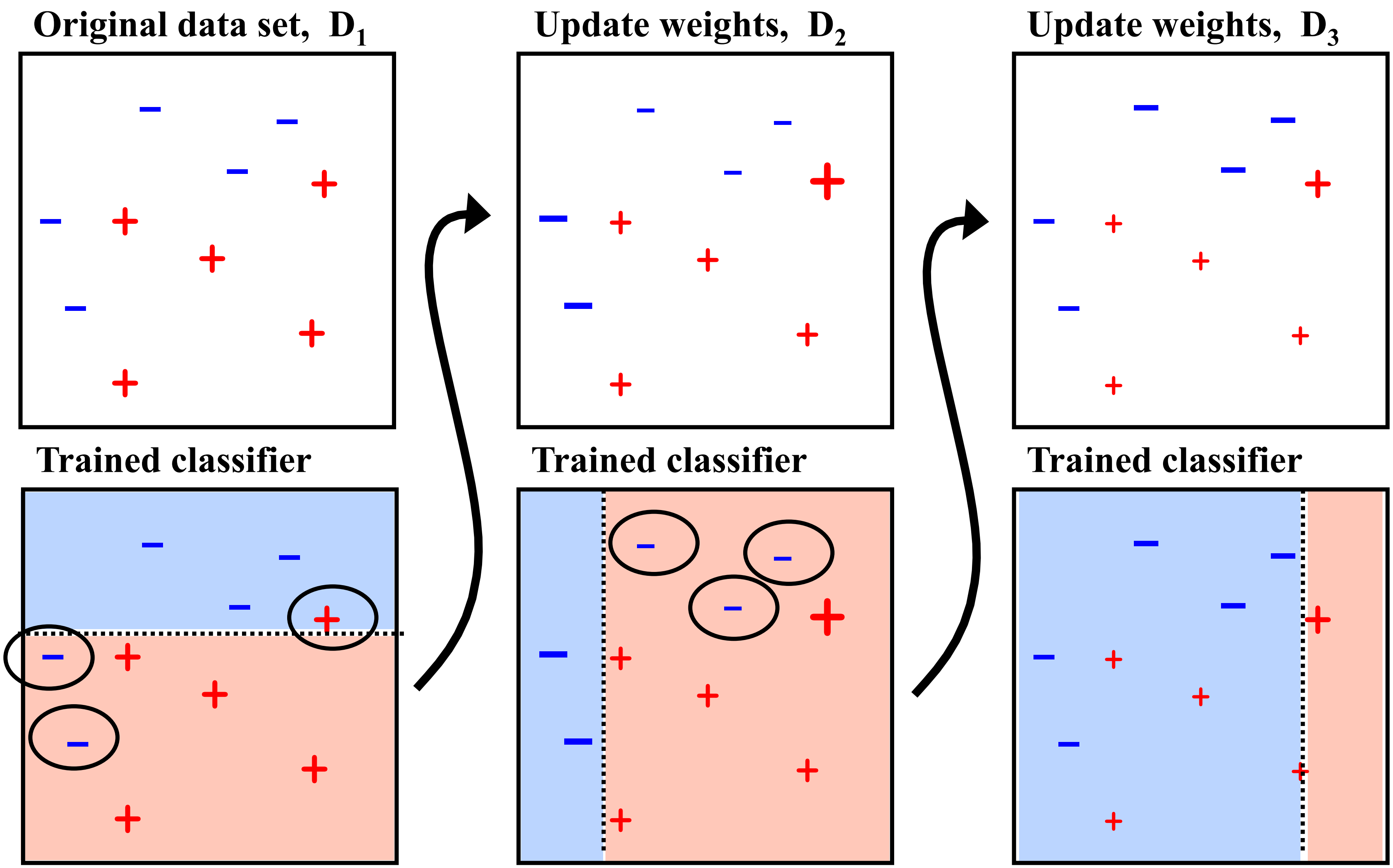
Boosting Example

Classes +1 , -1



Aside: minimizing weighted error

- So far we've mostly minimized unweighted error
- Minimizing weighted error is no harder:

Unweighted average loss:

$$J(\theta) = \frac{1}{N} \sum_i J_i(\theta, x^{(i)})$$

Weighted average loss:

$$J(\theta) = \sum_i w_i J_i(\theta, x^{(i)})$$

For any loss (logistic MSE, hinge, …)

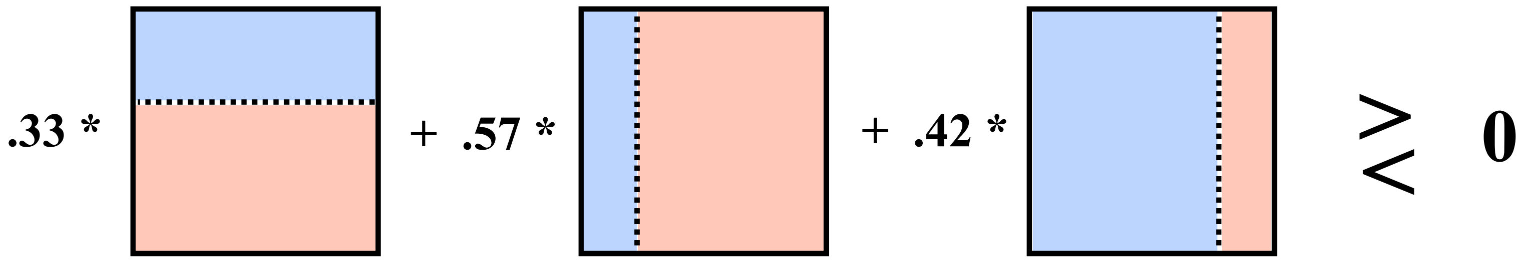
$$J(\theta, x^{(i)}) = \left(\sigma(\theta x^{(i)}) - y^{(i)}\right)^2$$

$$J(\theta, x^{(i)}) = \max\left[0\,,\ 1 - y^{(i)}\,\theta x^{(i)}\right]$$

For e.g. decision trees, compute weighted impurity scores:
p(+1) = total weight of data with class +1
p(-1) = total weight of data with class -1 => H(p) = impurity

Boosting Example

Weight each classifier and combine them:



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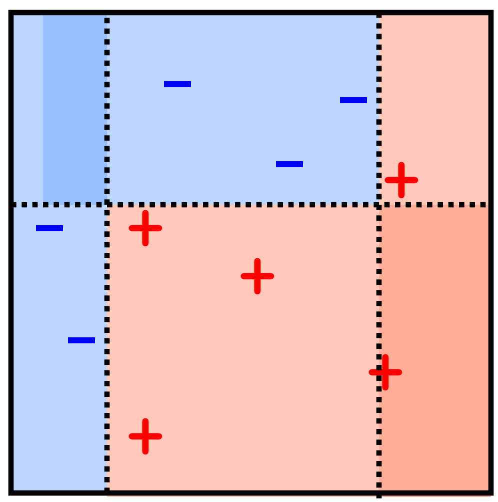
Combined classifier



1-node decision trees
“decision stumps”
very simple classifiers

AdaBoost = adaptive boosting

- Pseudocode for AdaBoost

Classes +1 , -1

```
for i=1:Nboost
  C{i} = train(X,Y,wts);         % Train a weighted classifier
  Yhat = predict(C{i},X);        % Compute predictions
  e = wts*(Y~=Yhat)';            % Compute weighted error rate
  alpha(i) = .5 log (1-e)/e;     % Compute coefficient
  wts *= exp(-alpha(i)*Y*Yhat);  % Update weights
  wts=wts/sum(wts);
 end;
 % Final classifier:
 ( \sum alpha(i)*predict(C{i},Xtest) ) > 0
```

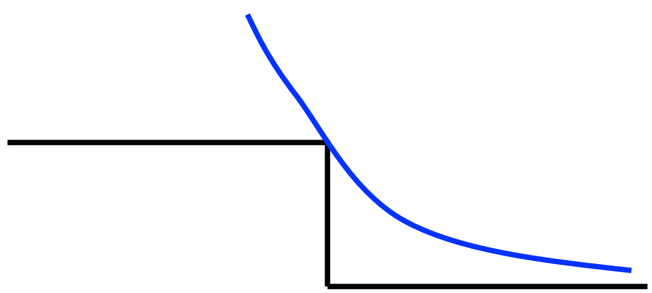
- Notes
  - e > .5 means classifier is not better than random guessing
  - Y * Yhat > 0 if Y == Yhat, and weights decrease
  - Otherwise, they increase

AdaBoost theory

- Minimizing classification error was difficult
  - For logistic regression, we minimized MSE instead
  - Idea: low MSE => low classification error
- Example of a surrogate loss function
- AdaBoost also corresponds to a surrogate loss f’ n

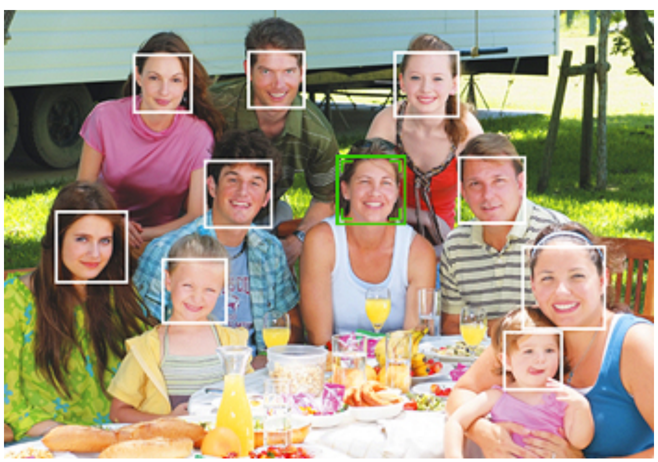
$$C_{ada} = \sum_i \exp[-y^{(i)} f(x^i)]$$

- Prediction is yhat = sign(f(x))
  - If same as y, loss < 1; if different, loss > 1; at boundary, loss=1
- This loss function is smooth & convex (easier to optimize)



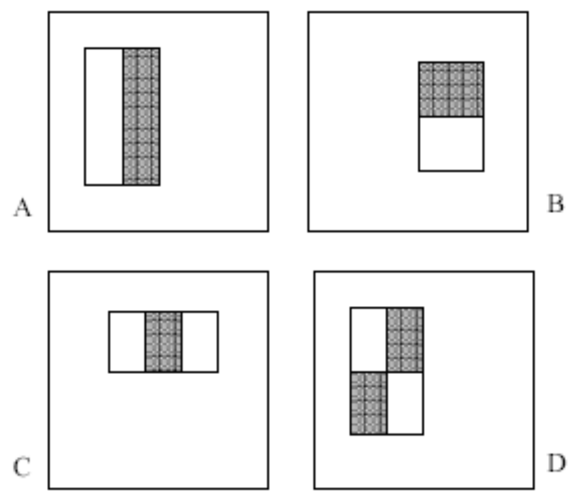
AdaBoost Example: Face Detection

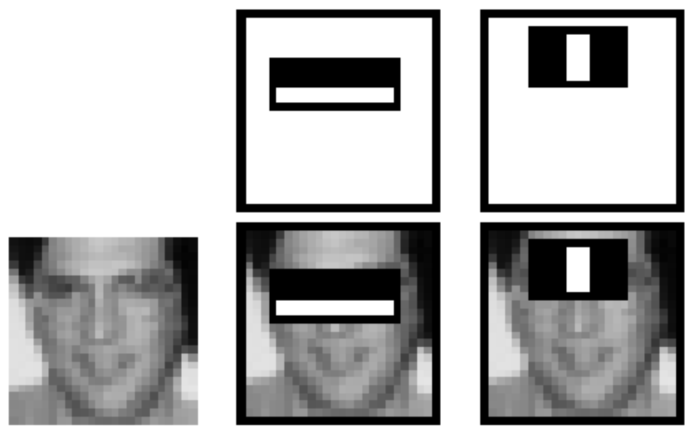
- Viola-Jones face detection algorithm
- Combine lots of very weak classifiers
  - Decision stumps = threshold on a single feature
- Define lots and lots of features
- Use AdaBoost to find good features
  - And weights for combining as well



Haar wavelet features

- Four basic types.
  - They are easy to calculate.
  - The white areas are subtracted from the black ones.
  - A special representation of the sample called the **integral image** makes feature extraction faster.





Training a face detector

- Wavelets give ~100k features
- Each feature is one possible classifier
- To train: iterate from 1:T
  - Train a classifier on each feature using weights
  - Choose the best one, find errors and re-weight

- This can take a long time… (lots of classifiers)
  - One way to speed up is to not train very well…
  - Rely on adaboost to fix "even weaker" classifier

- Lots of other tricks in "real" Viola-Jones
  - Cascade of decisions instead of weighted combo
  - Apply at multiple image scales
  - Work to make computationally efficient

Summary

- Ensemble methods
  - Combine multiple classifiers to make "better" one
  - Committees, majority vote
  - Weighted combinations
  - Can use same or different classifiers

- Boosting
  - Train sequentially; later predictors focus on mistakes by earlier

- Boosting for classification (e.g., AdaBoost)
  - Use results of earlier classifiers to know what to work on
  - Weight "hard" examples so we focus on them more
  - Example: Viola-Jones for face detection