Ensembles

• An ensemble is a set of classifiers whose combined results give the final decision.
MODEL* ENSEMBLES

• Basic Idea
  • Instead of learning one model
  • Learn several and combine them

• Often this improves accuracy by a lot

• Many Methods
  • Bagging
  • Boosting
  • Stacking

*A model is the learned decision rule. It can be as simple as a hyperplane in n-space (ie. a line in 2D or plane in 3D) or in the form of a decision tree or other modern classifier.
Bagging

• Generate bootstrap replicates of the training set by sampling with replacement

• Learn one model on each replicate

• Combine by uniform voting
Boosting

• Maintain a vector of weights for samples
• Initialize with uniform weights
• Loop
  – Apply learner to weighted samples
  – Increase weights of misclassified ones
• Combine models by weighted voting
Idea of Boosting
Boosting In More Detail
(Pedro Domingos’ Algorithm)

1. Set all E weights to 1, and learn H1.
2. Repeat m times: increase the weights of misclassified Es, and learn H2,…Hm.
3. H1..Hm have “weighted majority” vote when classifying each test
   Weight(H)=accuracy of H on the training data
ADABOOST

- ADABOOST boosts the accuracy of the original learning algorithm.

- If the original learning algorithm does slightly better than 50% accuracy, ADABOOST with a large enough number of classifiers is guaranteed to classify the training data perfectly.
/* First find the sum of the weights of the misclassified samples */
for j = 1 to N do /* go through training samples */
    if h[m](x_j) <> y_j then error <- error + w_j

/* Now use the ratio of error to 1-error to change the weights of the correctly classified samples */
for j = 1 to N do
    if h[m](x_j) = y_j then w[j] <- w[j] * error/(1-error)
Example

- Start with 4 samples of equal weight .25.
- Suppose 1 is misclassified. So error = .25.
- The ratio comes out .25/.75 = .33
- The correctly classified samples get weight of .25* .33 = .0825

What’s wrong? What should we do?

We want them to add up to 1, not .4975.

Answer: To normalize, divide each one by their sum (.4975).
Sample Application: Insect Recognition

Using circular regions of interest selected by an interest operator, train a classifier to recognize the different classes of insects.
Boosting Comparison

- **ADTree classifier only** (alternating decision tree)

- Correctly Classified Instances: 268 (70.1571 %)
- Incorrectly Classified Instances: 114 (29.8429 %)
- Mean absolute error: 0.3855
- Relative absolute error: 77.2229 %

<table>
<thead>
<tr>
<th>Classified as -&gt;</th>
<th>Hesperperla</th>
<th>Doroneuria</th>
</tr>
</thead>
<tbody>
<tr>
<td>Real</td>
<td>167</td>
<td>28</td>
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<tr>
<td>Hesperperlas</td>
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<td></td>
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<tr>
<td>Real</td>
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<td>136</td>
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<tr>
<td>Doroneuria</td>
<td></td>
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</tbody>
</table>
Boosting Comparison

AdaboostM1 with ADTree classifier

- Correctly Classified Instances: 303 (79.3194 %)
- Incorrectly Classified Instances: 79 (20.6806 %)
- Mean absolute error: 0.2277
- Relative absolute error: 45.6144 %

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<td>51</td>
<td>136</td>
</tr>
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</table>
Boosting Comparison

- RepTree classifier only *(reduced error pruning)*
  
  - Correctly Classified Instances  294  75.3846 %
  - Incorrectly Classified Instances  96  24.6154 %
  - Mean absolute error  0.3012
  - Relative absolute error  60.606  %

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<tr>
<td>Real Hesperperlas</td>
<td>169</td>
<td>41</td>
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<tr>
<td>Real Doroneuria</td>
<td>55</td>
<td>125</td>
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Boosting Comparison

AdaboostM1 with RepTree classifier

- Correctly Classified Instances: 324 (83.0769 %)
- Incorrectly Classified Instances: 66 (16.9231 %)
- Mean absolute error: 0.1978
- Relative absolute error: 39.7848 %

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<td>180</td>
<td>30</td>
</tr>
<tr>
<td>Real Doroneuria</td>
<td>36</td>
<td>144</td>
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</tbody>
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References


Stacking

- Apply multiple base learners (e.g.: decision trees, naive Bayes, neural nets)
- Meta-learner: Inputs = Base learner predictions
- Training by leave-one-out cross-validation: Meta-L. inputs = Predictions on left-out examples
Random Forests

- **Tree bagging** creates decision trees using the bagging technique. The whole set of such trees (each trained on a random sample) is called a decision forest. The final prediction takes the average (or majority vote).

- **Random forests** differ in that they use a modified tree learning algorithm that selects, at each candidate split, a random subset of the features.
Back to Stone Flies

Random forest of 10 trees, each constructed while considering 7 random features. Out of bag error: 0.2487. Time taken to build model: 0.14 seconds

Correctly Classified Instances 292 76.4398 % (81.4 with AdaBoost)
Incorrectly Classified Instances 90 23.5602 %
Kappa statistic 0.5272
Mean absolute error 0.344
Root mean squared error 0.4069
Relative absolute error 68.9062 %
Root relative squared error 81.2679 %
Total Number of Instances 382

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<th>F-Measure</th>
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<tr>
<td>WAvg.</td>
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<td>0.763</td>
<td>0.848</td>
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</table>

a b <-- classified as
129 58 | a = cal
32 163 | b = dor
More on Learning

• Neural Nets
• Support Vectors Machines
• Unsupervised Learning (Clustering)
  – K-Means
  – Expectation-Maximization
Neural Net Learning

• Motivated by studies of the brain.

• A network of “artificial neurons” that learns a function.

• Doesn’t have clear decision rules like decision trees, but highly successful in many different applications. (e.g. face detection)

• We use them frequently in our research.

$10^{11}$ neurons of > 20 types, $10^{14}$ synapses, 1ms–10ms cycle time
Signals are noisy “spike trains” of electrical potential
McCulloch–Pitts “unit”

Output is a “squashed” linear function of the inputs:

\[ a_i \leftarrow g(in_i) = g \left( \sum_j W_{j,i}a_j \right) \]

A gross oversimplification of real neurons, but its purpose is to develop understanding of what networks of simple units can do
(a) is a step function or threshold function

(b) is a sigmoid function $1/(1 + e^{-x})$

Changing the bias weight $W_{0,i}$ moves the threshold location
Simple Feed-Forward Perceptrons

\[ \text{in} = (\sum W_j x_j) + \theta \]
\[ \text{out} = g[\text{in}] \]

\( g \) is the activation function.
- It can be a step function: 
  \( g(x) = 1 \) if \( x \geq 0 \) and 0 (or -1) else.
- It can be a sigmoid function: 
  \( g(x) = \frac{1}{1+\exp(-x)} \).

The sigmoid function is differentiable and can be used in a gradient descent algorithm to update the weights.
Gradient Descent

takes steps proportional to the negative of the gradient of a function to find its local minimum

Let $X$ be the inputs, $y$ the class, $W$ the weights

- $\text{in} = \sum W_j \cdot x_j$
- $\text{Err} = y - g(\text{in})$
- $E = \frac{1}{2} \text{Err}^2$ is the squared error to minimize
- $\partial E / \partial W_j = \text{Err} \cdot \partial \text{Err} / \partial W_j = \text{Err} \cdot \partial / \partial W_j(g(\text{in}))(-1)$
- $= -\text{Err} \cdot g'(\text{in}) \cdot x_j$
- The update is $W_j \leftarrow W_j + \alpha \cdot \text{Err} \cdot g'(\text{in}) \cdot x_j$
- $\alpha$ is called the learning rate.
Simple Feed-Forward Perceptrons

repeat
  for each e in examples do
    in = (\sum W_j x_j) + \theta
    Err = y[e] - g[in]
    W_j = W_j + \alpha \cdot Err \cdot g'(in) \cdot x_j[e]
  until done

Examples: A=[(.5,1.5),+1], B=[(-.5,.5),-1], C=[(.5,.5),+1]
Initialization: W_1 = 1, W_2 = 2, \theta = -2

Note1: when g is a step function, the g'(in) is removed.
Note2: later in back propagation, Err * g'(in) will be called \Delta
Note3: We’ll let g(x) = 1 if x >=0 else -1
Graphically

Examples: A=[(.5,1.5),+1], B=[(-.5,.5),-1], C=[(.5,.5),+1]
Initialization: $W_1 = 1$, $W_2 = 2$, $\theta = -2$

Boundary is $W_1 x_1 + W_2 x_2 + \theta = 0$
Examples:
A=[(.5,1.5),+1],
B=[(-.5,.5),-1],
C=[(.5,.5),+1]
Initialization: W_1 = 1, W_2 = 2, \theta = -2

Let \alpha = .5

\[ W_1 \leftarrow W_1 + .5(2)(.5) \quad \text{leaving out } g' \]
\[ \quad \leftarrow 1 + 1(.5) = 1.5 \]

\[ W_2 \leftarrow W_2 + .5(2)(.5) \]
\[ \quad \leftarrow 2 + 1(.5) = 2.5 \]

\[ \theta \leftarrow \theta + .5(+1 - (-1)) \]
\[ \theta \leftarrow -2 + .5(2) = -1 \]
Graphically

Examples: A=[(.5,1.5),+1], B=[(-.5,.5),-1], C=[(.5,.5),+1]
Initialization: $W_1 = 1$, $W_2 = 2$, $\theta = -2$

Boundary is $W_1x_1 + W_2x_2 + \theta = 0$

approximately correct boundary
Apple/banana example

Training set:
\[
\begin{align*}
&\{ p_1 = \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix}, t_1 = (1) \} \\
&\{ p_2 = \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix}, t_2 = (0) \}
\end{align*}
\]

Initial weights:
\[
W = (0.5 - 1 - 0.5) \quad b = 0.5
\]

First iteration:
\[
\begin{align*}
&\quad a = \text{hardlim}(Wp_1 + b) = \text{hardlim} \left( (0.5 - 1 - 0.5) \times \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix} + 0.5 \right) \\
&\quad a = \text{hardlim}(-0.5) = 0 \\
&\quad e = t_1 - a = 1 - 0 = 1 \\
&\quad W^{new} = W^{old} + \eta p_1^T = (0.5 - 1 - 0.5) + (1)(-1 + 1 - 1) = (-0.5 + 0 - 1.5)
\end{align*}
\]

\[\eta = 1 \text{ in this example} \]
Second iteration

\[ a = \text{hardlim}(W_{p2} + b) = \text{hardlim} \left( \begin{pmatrix} -0.5 & 0 & -1.5 \end{pmatrix} \times \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} + 1.5 \right) \]

\[ a = \text{hardlim}(2.5) = 1 \quad e = t_2 - a = 0 - 1 = -1 \]

\[ W^{new} = W^{old} + ep^T \]

\[ W^{new} = (0.5 \ 0 \ -1.5) + (-1)(1 \ 1 \ -1) \]

\[ W^{new} = (-1.5 \ -1 \ -0.5) \]

\[ b^{new} = b^{old} + e = 1.5 + (-1) = 0.5 \]
Checking the solution (test vectors)

\[
a = \text{hardlim}(Wp_1 + b) = \text{hardlim}\left((1.5 - 1 - 0.5) \times \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix} + 0.5 \right)
\]

\[
a = \text{hardlim}(1.5) = 1 = t_1
\]

\[
a = \text{hardlim}(Wp_2 + b) = \text{hardlim}\left((1.5 - 1 - 0.5) \times \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} + 0.5 \right)
\]

\[
a = \text{hardlim}(-1.5) = 0 = t_2
\]
Checking the solution (testing the network)

\[ a = \text{hardlim} \left( (-1.5 - 1 - 0.5) \times \begin{pmatrix} -1 \\ 1 \\ -1 \end{pmatrix} + 0.5 \right) \]

\[ a = \text{hardlim}(1) = 1(\text{banana}) \]

\[ a = \text{hardlim} \left( (-1.5 - 1 - 0.5) \times \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} + 0.5 \right) \]

\[ a = \text{hardlim}(-2) = -1(\text{apple}) \]

The net recovers the correct answer from noisy information:

\[ a = \text{hardlim} \left( (-1.5 - 1 - 0.5) \times \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix} + 0.5 \right) \]

\[ a = \text{hardlim}(3) = 1(\text{banana}) \]
Back Propagation

• Simple single layer networks with feed forward learning were not powerful enough.
• Could only produce simple linear classifiers.
• More powerful networks have multiple hidden layers.
• The learning algorithm is called back propagation, because it computes the error at the end and propagates it back through the weights of the network to the beginning.
The backpropagation algorithm

The following is the backpropagation algorithm for learning in multilayer networks.

function BACK-PROP-LEARNING(examples, network)
returns a neural network

inputs:
examples, a set of examples, each with input vector \( x \) and output vector \( y \).
network, a multilayer network with \( L \) layers, weights \( W_{j,i} \), activation function \( g \)
locally defined variables: \( \Delta \), a vector of errors, indexed by network node

for each weight \( w_{i,j} \) in network do
    \( w_{i,j} \) ← a small random number
repeat
    for each example \((x, y)\) in examples do
        /* Propagate the inputs forward to compute the outputs. */
        for each node \( i \) in the input layer do  // Simply copy the input values.
            \( a_i \) ← \( x_i \)
        for \( l = 2 \) to \( L \) do  // Feed the values forward.
            for each node \( j \) in layer \( l \) do
                \( in_j \) ← \( \sum_i w_{i,j} a_i \)
                \( a_j \) ← \( g(in_j) \)
        for each node \( j \) in the output layer do  // Compute the error at the output.
            \( \Delta[j] \) ← \( g'(in_j) \times (y_j - a_j) \)
        /* Propagate the deltas backward from output layer to input layer */
        for \( l = L - 1 \) to \( 1 \) do
            for each node \( i \) in layer \( l \) do
                \( \Delta[i] \) ← \( g'(in_i) \sum_j w_{i,j} \Delta[j] \)  // “Blame” a node as much as its weight.
        /* Update every weight in network using deltas. */
        for each weight \( w_{i,j} \) in network do
            \( w_{i,j} \) ← \( w_{i,j} + \alpha \times a_i \times \Delta[j] \)  // Adjust the weights.
    until some stopping criterion is satisfied

return network
The backpropagation algorithm

The following is the backpropagation algorithm for learning in multilayer networks.

function BACK-PROP-LEARNING(examples, network) returns a neural network

inputs:

examples, a set of examples, each with input vector $x$ and output vector $y$.

network, a multilayer network with $L$ layers, weights $W_{j,i}$, activation function $g$

local variables: $\Delta$, a vector of errors, indexed by network node

for each weight $w_{i,j}$ in network do

$w_{i,j} \leftarrow$ a small random number

layer 1  2  3=L

x1 w11 n1 w1f nf
x2 w21 n1 w2f
x3 w31 n2
repeat
  for each example \((x,y)\) in examples do
    /* Propagate the inputs forward to compute the outputs. */
    for each node \(i\) in the input layer do        // Simply copy the input values.
      \(a_i \leftarrow x_i\)
    for \(l = 2\) to \(L\) do
      for each node \(j\) in layer \(l\) do          // Feed the values forward.
        \(\text{in}_j \leftarrow \sum_i w_{i,j} a_i\)
        \(a_j \leftarrow g(\text{in}_j)\)
for each node \( j \) in the output layer do

\[
\Delta[j] \leftarrow g'(in_j) \times (y_j - a_j)
\] // Compute the error at the output.

- Node \( nf \) is the only node in our output layer.
- Compute the error at that node and multiply by the derivative of the weighted input sum to get the change delta.
/* Propagate the deltas backward from output layer to input layer */
for \( l = L - 1 \) to 1 do
  for each node \( i \) in layer \( l \) do
    \[ \Delta[i] \leftarrow g'(i_n_i) \sum_j w_{i,j} \Delta[j] \]  // “Blame” a node as much as its weight

• At each of the other layers, the deltas use
  • the derivative of its input sum
  • the sum of its output weights
  • the delta computed for the output error
Now that all the deltas are defined, the weight updates just use them.
Back Propagation Summary

• Compute delta values for the output units using observed errors.

• Starting at the output-1 layer
  – repeat
    • propagate delta values back to previous layer
    • update weights between the two layers
  – till done with all layers

• This is done for all examples and multiple epochs, till convergence or enough iterations.
Time taken to build model: 16.2 seconds

Correctly Classified Instances 307  80.3665 % (did not boost)
Incorrectly Classified Instances  75  19.6335 %
Kappa statistic 0.6056
Mean absolute error 0.1982
Root mean squared error 0.41
Relative absolute error 39.7113 %
Root relative squared error 81.9006 %
Total Number of Instances 382

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<tr>
<td>0.706</td>
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<tr>
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<td>0.897</td>
<td>0.824</td>
<td>0.872</td>
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</table>
W Avg. 0.804 0.2  0.814 0.804 0.802 0.872

=== Confusion Matrix ===

<table>
<thead>
<tr>
<th>a</th>
<th>b</th>
</tr>
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<tbody>
<tr>
<td>a = cal</td>
<td>132 55</td>
</tr>
<tr>
<td>b = dor</td>
<td>20 175</td>
</tr>
</tbody>
</table>
Handwritten digit recognition

0 1 2 3 4 5 6 7 8 9
0 1 2 3 4 5 6 7 8 9

3-nearest-neighbor = 2.4% error
400–300–10 unit MLP = 1.6% error
LeNet: 768–192–30–10 unit MLP = 0.9% error

Current best (kernel machines, vision algorithms) $\approx 0.6\%$ error