Nonlinear Classifiers I

Nonlinear Classifiers: Introduction

- Road map

[Diagram showing the road map with steps: Preprocessing, Feature extraction, Classification, and two classes: "salmon", "sea bass"]
Nonlinear Classifiers: Introduction

- Classifiers
  - Supervised Classifiers
    - Linear Classifiers
      - Perceptron
      - Least Squares Methods
      - Linear Support Vector Machine
  - **Nonlinear Classifiers**
    - Part I: Multi Layer Neural Networks
    - Part II: Nonlinear Support Vector Machine
  - Decision Trees
  - Unsupervised Classifiers

An example: Suppose we’re in 1-dimension

What would a linear SVMs do with this data?
Nonlinear Classifiers: Introduction

• An example: Suppose we’re in 1-dimension

Not a big surprise

• Harder 1-dimensional dataset

What can be done about this?
Nonlinear Classifiers: Introduction

non-linear basis function

\[ z_k = (x_k, x_k^2) \]
Nonlinear Classifiers: Introduction

- **Linear classifiers** are simple and computationally efficient.
- However for nonlinearly separable features, they might lead to very inaccurate decisions.
- Then we may trade simplicity and efficiency for accuracy using a **nonlinear classifier**.

Nonlinear Classifiers: Agenda

Part I: Nonlinear Classifiers

Multi Layer Neural Networks
- XOR problem
- Two-Layer Perceptron
- Backpropagation
- Choice of the network size
- Model selection techniques
- Applications: XOR, ZIP Code, OCR problem
- Demo: SNNS, BPN
Nonlinear Classifiers: Agenda

Part I: Nonlinear Classifiers

Multi Layer Neural Networks

- **XOR problem**
- **Two-Layer Perceptron**
- Backpropagation
- Choice of the network size
- Model selection techniques
- Applications: XOR, ZIP Code, OCR problem
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The XOR problem

<table>
<thead>
<tr>
<th>$x_1$</th>
<th>$x_2$</th>
<th>XOR</th>
<th>Class</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>B</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>A</td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>1</td>
<td>A</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>0</td>
<td>B</td>
</tr>
</tbody>
</table>

- There is no single line (hyperplane) that separates class A from class B. On the contrary, AND and OR operations are linearly separable problems.
The Two-Layer Perceptron

• For the XOR problem, draw two lines, instead of one.

• Then class B is outside the shaded area and class is A inside.

• We call it a two-step design.

The Two-Layer Perceptron

• Step 1: Draw two lines (hyperplanes)

\[ g_1(x) = 0, \]
\[ g_2(x) = 0 \]

Each of them is realized by a perceptron. The outputs of the perceptrons will be

\[ y_i = f( g_i(x) ) = \begin{cases} 0 & i = 1, 2 \\ 1 & \end{cases} \]

depending on the value of \( x \) (\( f \) is the activation function).

• Step 2: Find the ‘position’ of \( x \) w.r.t. both lines, based on the values of \( y_1, y_2 \).
The Two-Layer Perceptron

- Equivalently:
  1. The computations of the first step perform a mapping
     \[ x \rightarrow y = [y_1, y_2]^T \]
  2. The decision is then performed on the transformed data \( y \).

<table>
<thead>
<tr>
<th>1st step</th>
<th>2nd step</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 0 0(-) 0(-)</td>
<td>B(0)</td>
</tr>
<tr>
<td>0 1 1(+) 0(-)</td>
<td>A(1)</td>
</tr>
<tr>
<td>1 0 1(+) 0(-)</td>
<td>A(1)</td>
</tr>
<tr>
<td>1 1 1(+) 1(+)</td>
<td>B(0)</td>
</tr>
</tbody>
</table>

The Two-Layer Perceptron

- This decision can be performed via a second line \( g(y) = 0 \), which can also be realized by a perceptron.

- Computations of the first step perform a mapping that transforms the nonlinearily separable problem to a linearly separable one.
The Two-Layer Perceptron

- The architecture

This is known as the two layer perceptron with one hidden and one output layer. The activation functions are:

\[
f(x) = \begin{cases} 
1 & x \geq 0 \\
0 & x < 0
\end{cases}
\]

- The nodes (neurons) of the figure realize the following lines (hyper planes).

\[
g_1(x) = 1x_1 + 1x_2 - \frac{1}{2} = 0 \\
g_2(x) = 1x_1 + 1x_2 - \frac{2}{3} = 0 \\
g_3(y) = 1y_1 - 2y_2 - \frac{1}{2} = 0
\]

- Classification capabilities:
All possible mappings performed by the first layer are onto the vertices of the unit side square, e.g., (0, 0), (1, 0), (1, 0), (1, 1).
Classification capabilities

- The more general case
  \( \mathbf{x} \in \mathbb{R}^l \),
  \( y_i \in \{0, 1\} \quad i = 1, 2, \ldots, p \)
  \( \mathbf{x} \rightarrow \mathbf{y} = [y_1, \ldots, y_p]^T, \quad \mathbf{y} \in \mathbb{R}^r \)
  \( y_i = f(g_i) \)

\[
g_i(x) = \sum_{k=1}^{i} w_{ik} x_k + w_{i0} = 0
\]
\[
g_j(y) = \sum_{k=1}^{j} w_{jk} y_k + w_{j0} = 0
\]

- performs a mapping of a vector onto the vertices of the unit side \( H_p \) hypercube.

Classification capabilities

- The mapping is achieved with \( p \) nodes each realizing a hyperplane. The output of each of these nodes is 0 or 1 depending on the relative position of \( \mathbf{x} \) w.r.t. the hyperplane.

Intersections of these hyperplanes form regions in the \( l \)-dimensional space. Each region corresponds to a vertex of the \( H_p \) unit hypercube.
Classification capabilities

For example, the 001 vertex corresponds to the region which is located to the (-) side of \( g_1(x) = 0 \) to the (-) side of \( g_2(x) = 0 \) to the (+) side of \( g_3(x) = 0 \).

The output node realizes a hyperplane in the \( y \) space, that separates some of the vertices from the others. Thus, the two layer perceptron has the capability to classify vectors into classes that consist of unions of polyhedral regions. But not ANY union. It depends on the relative position of the corresponding vertices.

The Three-Layer Perceptron

- This is capable to classify vectors into classes consisting of ANY union of polyhedral regions.
- The idea is similar to the XOR problem. It realizes more than one plane in the space.
The reasoning

- For each vertex, corresponding to class A, construct a hyperplane which leaves **THIS vertex** on one side (+) and **ALL** the others to the other side (-).

- The output neuron realizes an OR gate.

Overall:

The first layer of the network forms the **hyperplanes**, the second layer forms the **regions** and the output nodes forms the **classes**.

The Multi-Layer Neural Network

![Diagram of Multi-Layer Neural Network]

for the i-th trainings pair

\[ y^{r-1}_k(i) \text{ output of the } k\text{-th node at layer } r-1 \]

\[ v^r_j(i) \text{ argument for } f(\cdot) \text{ for the } i\text{-th trainings pair} \]

\[ v^r_j(i) = \sum_{k=0}^{K-1} w^r_{jk} y^{r-1}_k(i) + w^r_{jo} = \sum_{k=0}^{K-1} w^r_{jk} y^{r-1}_k(i), \text{ with } y^r_{jo}(i) = +1 \]

\[ v^r_j(i) = w^r_{jo} y^{r-1}_j(i) \]

\[ y^r_j(\cdot) = f(v^r_j(i)) = f \left( w^r_{jo} y^{r-1}_j(i) \right) \]
Nonlinear Classifiers: Agenda

Part I: Nonlinear Classifiers

Multi Layer Neural Networks
- XOR problem
- Two-Layer Perceptron
- **Backpropagation algorithm to train multilayer perceptrons**
- Choice of the network size
- Model selection techniques
- Applications: XOR, ZIP Code, OCR problem
- Demo: SNNS, BPN

The Backpropagation Algorithm (BP)

- Designing Multilayer Perceptrons
  - One direction is to adopt the above rationale and develop a structure that classifies correctly all the training patterns.
  - The other direction is to choose a structure and compute the $w$’s, often called ‘synaptic weights’, to optimize a cost function.
  - BP is an algorithmic procedure that computes the synaptic weights iteratively, so that an adopted cost function is minimized (optimized).
The Backpropagation Algorithm

The Steps:

1. Adopt an optimizing cost function $J(i)$, e.g.,
   - Least Squares Error
   - Relative Entropy

   between desired responses and actual responses of the network for the available training patterns.

   ➔ That is, from now on we have to live with errors. We only try to minimize them, using certain criteria.

2. Adopt an algorithmic procedure for the optimization of the cost function with respect to the weights $w$ e.g.:
   - Gradient descent
   - Newton’s algorithm
   - Conjugate gradient
The Backpropagation Algorithm

The Steps:

3. The task is a **nonlinear** optimization e.g. with gradient descent.

\[ w_{j}^{r}(\text{new}) = w_{j}^{r}(\text{old}) + \Delta w_{j}^{r} \]

\[ \Delta w_{j}^{r} = -\mu \frac{\partial J}{\partial w_{j}^{r}} \]

\[ J = \sum_{i=1}^{N} E(i) \]

BackProp: Step 3 nonlinear optimization

Detail: Computation of the Gradients.

\[ w_{j}^{r}(\text{new}) = w_{j}^{r}(\text{old}) + \Delta w_{j}^{r} \]

\[ \Delta w_{j}^{r} = -\mu \frac{\partial J}{\partial w_{j}^{r}} \]

\[ \frac{\partial E}{\partial w_{j}^{r}} = \frac{\partial E}{\partial u_{j}^{r}(i)} \frac{\partial u_{j}^{r}(i)}{\partial w_{j}^{r}} \]

\[ \frac{\partial E}{\partial u_{j}^{r}(i)} = \delta_{j}^{r}(i) \]

\[ \Delta w_{j}^{r} = -\mu \sum_{i=1}^{N} \delta_{j}^{r}(i) y_{i}^{r-1}(i) \]
BackProp: Step 3 nonlinear optimization

Detail: Computation of $\delta_j^r(i)$ for Least Squares

**Case $r = L$ (Last Layer)**

$$\delta_j^L(i) = \frac{\partial E}{\partial u_j^L(i)} \Rightarrow \delta_j^L = e_j(i) f'(u_j^L(i))$$

**Case $r < L$**

$$\delta_j^{r-1}(i) = \sum_{k=1}^{m} \frac{\partial E}{\partial v_{jk}^{r-1}(i)} \frac{\partial v_{jk}^{r-1}(i)}{\partial u_j^r(i)}$$

$$\delta_j^{r-1}(i) = \left[ \sum_{k=1}^{m} \delta_k^L(i) w_{kj}^r \right] f'(u_j^{r-1}(i))$$

$$\Rightarrow \delta_j^{r-1}(i) = e_j^{r-1}(i) f'(u_j^{r-1}(i))$$

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BackProp: Step 3 summary

3. The task is a **nonlinear** optimization.

**e.g.** gradient descent.

$$w_j^r(\text{new}) = w_j^r(\text{old}) + \Delta w_j^r$$

$$\Delta w_j^r = -\mu \frac{\partial J}{\partial w_j^r}$$

with the following up-date rules:

$$\Delta w_j^r = -\mu \sum_{i=1}^{N} \delta_j^L(i) y_j^{r-1}(i)$$

Error $e_j(i)$: Difference of actual and desired response for the $j$-th output neuron

$$e_j(i) = y_j^r(i) - \hat{y}_j(i)$$

$$\delta_j^L(i) = e_j(i) f'(u_j^L(i))$$

$$\delta_j^{r-1}(i) = \left[ \sum_{k=1}^{m} \delta_k^r(i) w_{kj}^r \right] f'(u_j^{r-1}(i))$$
The Backpropagation Algorithm

The Procedure:

1. **Initialization:**
   Initialize unknown weights randomly with small values.

2. **Forward computations:**
   For each of the training examples compute the output of all neurons of all layers. Compute the cost function for the current estimate of weights.

3. **Backward computations:**
   Compute the gradient terms backwards, starting with the weights of the last (e.g. 3rd) layer and then moving towards the first.

4. **Update:** Update the weights.

5. **Termination:**
   Repeat until a termination procedure is met.

The Backpropagation Algorithm

- In a large number of optimizing procedures, computation of derivatives are involved. Hence, discontinuous activation functions pose a problem, i.e.,

\[
f(x) = \begin{cases} 
1 & x > 0 \\
0 & x < 0 
\end{cases}
\]

- There is always an escape path!!! e.g. the logistic function:

\[
f(x) = \frac{1}{1 + \exp(-ax)}
\]

\[
f'(x) = \alpha f(x)(1 - f(x))
\]

Other differentiable functions are also possible and in some cases more desirable.
The Backpropagation Algorithm

Two major philosophies:

- **Batch mode:** The gradients of the last layer are computed once ALL training data have appeared to the algorithm, i.e., by summing up all error terms.

- **Pattern mode:** The gradients are computed every time a new training data pair appears. Thus gradients are based on successive individual errors.

The Backpropagation Algorithm

A major problem:
The algorithm may converge to a local minimum.

The cost function choice
Examples:
- **The Least Squares**

\[
J = \sum_{i=1}^{N} E(i)
\]

\[
E(i) = \frac{1}{2} \sum_{m=1}^{K} e_m^2(i) = \frac{1}{2} \sum_{m=1}^{K} (y_m(i) - \hat{y}_m(i))^2 \\
i = 1, 2, ..., N
\]

\[\hat{y}_m(i) : \text{ Desired response of } m\text{-th output node (1 or 0) for input } x(i).\]

\[y_m(i) : \text{ Actual response of } m\text{-th output node, in the interval } [0, 1], \text{ for input } x(i).\]
The Backpropagation Algorithm

The cost function choice

Examples:

• The cross-entropy

\[ J = \sum_{i=1}^{N} E(i) \]

\[ E(i) = \sum_{m=1}^{k} \left( y_m(i) \ln \hat{y}_m(i) + (1 - y_m(i)) \ln (1 - \hat{y}_m(i)) \right) \]

This presupposes an interpretation of \( y \) and \( \hat{y} \) as probabilities!

Classification error rate:

• Also known as discriminative learning.

• Most of these techniques use a smoothed version of the classification error.

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The Backpropagation Algorithm

“Well formed” cost functions:

• Danger of local minimum convergence.

• “Well formed” cost functions guarantee convergence to a “good” solution.

• That is one that classifies correctly ALL training patterns, provided such a solution exists.

• The cross-entropy cost function is a well formed one. The Least Squares is not.
The Backpropagation Algorithm

**optimally class a-posteriori probabilities:**

Both, the Least Squares and the cross entropy lead to output values \( \hat{y}_m(i) \) that approximate optimally class a-posteriori probabilities!

\[
\hat{y}_m(i) \approx P(\omega_m \mid x(i))
\]

That is, the probability of class \( \omega_m \) given \( x(i) \).

- It does not depend on the underlying distributions!!! It is a characteristic of certain cost functions and the chosen architecture of the network. It depends on the model how good or bad the approximation is.

- It is valid at the global minimum.

Nonlinear Classifiers: Agenda

Part I: Nonlinear Classifiers

Multi Layer Neural Networks
- XOR problem
- Two-Layer Perceptron
- Backpropagation
  - **Choice of the network size**
    - Number of layers and of neurons per layer
    - Model selection techniques
      - Pruning techniques
      - Constructive techniques
- Applications: XOR, ZIP Code, OCR problem
- Demo: SNNS, BPN
Choice of the network size

How big a network can be. How many layers and how many neurons per layer?
There are two major techniques:

- **Pruning Techniques:**
  These techniques start from a large network and then weights and/or neurons are removed iteratively, according to a criterion.

- **Constructive techniques:**
  They start with a small network and keep increasing it, according to a predetermined procedure and criterion.

Choice of the network size

- **Pruning Techniques:**
  - Methods based on parameter sensitivity

  \[
  \delta J = \sum_i g_i \delta w_i + \frac{1}{2} \sum_i h_i \delta w_i^2 + \frac{1}{2} \sum_i \sum_i h_i \delta w_i \delta w_j
  \]

  + higher order terms where

  \[
  g_i = \frac{\partial J}{\partial w_i}, \quad h_i = \frac{\partial^2 J}{\partial w_i \partial w_j}
  \]

  Near a minimum and assuming \( \delta J \approx \frac{1}{2} \sum h_i \delta w_i^2 \)

  Pruning is now achieved as:

  1. Train the network using Backpropagation for a number of steps
  2. Compute the saliencies

  \[
  s_i = \frac{h_i w_i^2}{2}
  \]

  3. Remove weights \( w_i \) with small \( s_i \).
  4. Repeat the process
Choice of the network size

Idea: Start with a large network and leave the algorithm to decide which weights are small.

Generalization properties:
- Large network learn the particular details of the training set.
- Not be able to perform well when presented with data unknown to it.

=> The size of the network must be:
- Large enough to learn what makes data of the same class similar and data from different classes dissimilar.
- Small enough not to be able to learn underlying differences between data of the same class. This leads to the so called overfitting.

Choice of the network size

Example:
- Decision curve (a) before and (b) after pruning.
Choice of the network size

Overtraining is another side of the same coin, i.e., the network adapts to the peculiarities of the training set.

Nonlinear Classifiers: Conclusion

Part I: Nonlinear Classifiers

Multi Layer Neural Networks

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- Backpropagation
- Choice of the network size
- Model selection techniques

- Applications: XOR, ZIP Code, OCR problem
- Demo: SNNS, BPN
Nonlinear Classifiers: Conclusion

- **Applications:** XOR, ZIP Code, OCR problem
- **Demo:** Java-NNS, BPN

http://www-ra.informatik.uni-tuebingen.de/downloads/JavaNNS/

Nonlinear Classifiers: Outlook

Part II: Nonlinear Classifiers

- Polynomial Classifier
  - Special case of a Two-Layer Perceptron
  - Activation function is an exponent function
- Radial Basis Function Network
  - Special case of a two-layer network
  - Radial Basis activation Function
  - Training is simpler and faster
- Nonlinear SVM
  - Application: ZIP Code, OCR problem
    - Improvement given by the nonlinearity.
  - Demo: libSVM, DHS or Hlavac