

## Chapter 9

# Applications in Bioinformatics and Medical Informatics

This chapter presents two interesting applications of PSO in bioinformatics and medical informatics. The first consists of the adaptation of probabilistic neural network models for medical classification tasks. The second application employs the unified PSO algorithm to tackle magnetoencephalography problems. Our main goal is to clarify crucial points where PSO interferes with the employed computational models and provide details on the formulation of the corresponding optimization problems and experimental settings. Indicative results are reported to illustrate the workings of the algorithms and provide representative samples of their performance.

### INTRODUCTION

The research blossoming of the past few years in molecular biology and brain studies has produced a huge amount of data. The need for their processing and assessment gave rise to the field of *bioinformatics*, which deals with the application of information processing methodologies on biological and biomedical tasks. This includes data handling, as well as the development of computational models for the better understanding of the studied physical systems. Modeling, data mining and machine learning occupy a central place in bioinformatic research, which tackles problems such as protein localization, sequence and genome analysis, brain activity monitoring and analysis etc.

Different methodologies have been proposed to address the aforementioned problems. Artificial neural networks, evolutionary algorithms and swarm intelligence are considered among the most popular methodologies today, thanks to their efficiency in analyzing and extracting knowledge from systems with inherent non-deterministic structure and responses. In this chapter, we present two applications

where PSO is used in combination with different modeling techniques to tackle challenging biomedical problems.

The first application refers to the adaptation of probabilistic neural networks (Georgiou *et al.*, 2006). A self-adaptive model is considered, where PSO serves as its basic configuration mechanism. The resulting model is applied on two protein localization problems, as well as on two medical diagnostic tasks, with very promising results. The second application comes from the field of brain studies and refers to the solution of source localization problems in magnetoencephalography (Parsopoulos *et al.*, 2009). In this case, PSO is employed to detect an unknown excitation source, using only a number of sensor measurements. As a second task, we consider the detection of proper parameters in established spherical expansion models. Such models are used in brain studies for the approximation of the brain magnetic potential. A representative portion of published results for both applications are reported and discussed to justify the usefulness of PSO and probe its potential for addressing similar applications.

## **CALIBRATING PROBABILISTIC NEURAL NETWORKS**

*Probabilistic neural networks* (PNNs) are supervised classification neural network models, closely related to the Bayes classification rule and the Parzen nonparametric probability density function estimation theory (Parzen, 1962; Specht, 1990). Their main advantage against different classifiers is their ability to effectively exploit all the available information on the problem at hand and provide uncertainty measures of the classification accuracy. For example, in a cancer classification task, PNNs can estimate the probability of a tumor being benign or malignant, instead of the yes/no responses provided by most classifiers.

PNNs have been used in a plethora of bioinformatics and medical tasks. Huang (2002) presents a comprehensive study of PNNs combined with a feature extraction method on cancer classification problems. Holmes *et al.* (2001) used PNNs to develop accurate NMR-based metabonomic models for the prediction of xenobiotic-induced toxicity in experimental animals, emphasizing their potential use in accelerated drug discovery programs. Guo *et al.* (2004) considered PNNs for the design of an automatic, reliable, and efficient prediction system for protein subcellular localization in large-scale genome analysis, while Wang *et al.* (1998) used PNNs to identify subtle changes in brain tissue quantities and volumes through magnetic resonance image analysis.

The classification capabilities of PNNs can be attributed to inherent properties stemming from their originating methodologies, namely statistical pattern recognition and artificial NNs. Actually, PNNs constitute a NN implementation of kernel discriminant analysis that employs Bayesian strategies for pattern classification. Each pattern is stored as a separate neuron in the PNN; thus, it can be viewed as an “intelligent” memory (Berthold & Diamond, 1998). This feature results in lower execution time and straightforward training but also in higher storage requirements than the typical feedforward NNs. The next section describes the basics on PNNs.

### **Probabilistic Neural Networks**

The structure of a PNN is similar to that of feedforward NNs, described in Chapter Six. However, they always have only four layers, named as *input*, *pattern*, *summation*, and *output layer*, respectively, as illustrated in Fig. 1. Let the problem at hand consist of  $K$  classes with  $M_k$  training patterns per class,  $k =$

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