CHAPTER 1

Introduction

1. Computational Ecology

Ecology is the scientific study of the relationship between organisms and their environments. This concept was put forward by Haeckel as early as 1866. Through more than one hundred years' development, ecology has become a major branch of knowledge. This is especially so since the early 1990s: ecology has evolved to be one of the centers of modern science.

There are many sub-disciplines of ecology. Depending on the organizational levels of organisms, ecology is divided into molecular ecology, physiological ecology, population ecology, community ecology, ecosystems ecology, landscape ecology, etc.; according to the differences in taxa categories of organisms, there are plant ecology, animal ecology, microbial ecology, insect ecology, etc.; based on the differences in landscape and habitat categories, there are terrestrial ecology, marine ecology, wetland ecology, or forest ecology, grassland ecology, etc.; if we focus on application categories, they are agro-ecology, urban ecology, pollution ecology, etc., and if we categorize in terms of scientific disciplines, there are mathematical ecology, environmental ecology, chemical ecology, physiological ecology, economic ecology, behavioral ecology, etc.

Among the known ecological disciplines, only mathematical ecology is a pure quantitative science. Mathematical ecology stresses the mathematical analysis of ecological issues, mostly by developing analytical models and equations.

Due to the complexity, nonlinearity and uncertainty of ecological problems, simple mathematical models or equations are far from enough to address them. As the knowledge of ecology and computational science advances, intensive computation is playing an increasingly important role in ecological studies. Various theories and methods based on intensive computation, like artificial neural networks, agent-based modeling, systems simulation, numerical approximation, etc., are increasingly used in ecology. As a result, an ecological discipline, computational ecology, is formally proposed here to integrate, synthesize and promote computation-intensive areas in ecology.

Research tasks in the discipline of computational ecology are described below:

(1) Computational ecology is a science focusing mainly on ecological researches, constructions and applications of theories and methods of computational science including computational mathematics. Intensive computation is one of the major features of computational ecology. Most of the issues in computational ecology start from modeling, followed by intensive computation based on the model (iteration, training, etc.). It aims at the simulation, approximation, prediction, recognition, and classification of ecological issues. With computational ecology as a unified platform, we may not only apply theories and methods of computational science to ecology, but also construct new theories and methods for computational science. It is an interface, membrane, or gate between ecology and computational science.
(2) Ecology is the main body of computational ecology. Various sciences are involved in computational ecology, including computational mathematics (such as numerical methods), artificial intelligence (artificial neural networks, machine learning, etc.), computer science (algorithm design, software development, etc.), probability theory, statistics, optimization theory, combinatorics, differential equations, functional analysis, algebraic topology, differential geometry, and others.
(3) The research areas of computational ecology involve (but not limited to) the following aspects:

    (a) Artificial neural networks, knowledge-based systems, machine learning, data exploration, statistical computation (Bayesian computing, randomization, bootstrapping, Monte Carlo techniques, stochastic process, etc.), computation-intensive inferential methods, heuristics, numerical and optimization methods, individual-based modeling and simulation (differential and difference equation modeling and simulation, etc.), prediction, recognition, classification, agent-based modeling and simulation, network analysis and computation, databases, and other computation-intensive theories and methods.

(b) The development, evaluation and validation of software and algorithms for computational ecology. The development and evaluation of apparatus, instruments and machines for ecological and environmental analysis, investigation and monitoring based on the software of computational ecology.

2. Artificial Neural Networks and Ecological Applications

2.1. *A brief history of artificial neural networks*

An artificial neural network is a simulation system of human brain. It can be implemented by both electric elements and computer software. It is a parallel distributed processor with large numbers of connections. Artificial neural networks can achieve knowledge by learning and possess the ability of problem-solving, and the knowledge achieved is stored in connection weights.

Researches on modern artificial neural networks began approximately 60 years ago. Development of artificial neural networks has undergone four phases (Fecit, 2003).

(1) **Birth phase.** As early as 1943, McCulloch and Pitts described a neural network with mathematical tools and presented the mathematical model of neurons, i.e., MP model. MP model was finally developed to the theory of limited automata. Their works demonstrated that artificial neural networks can be used to compute any arithmetic and logic functions. Their works were recognized as the origination of artificial neural network researches.

In 1949 Hebb speculated that the conditioned response resulted from the characteristics of single neuron. He thus presented a hypothesis on the learning law of neurons. The hypothesis was proved in the following 30 years and widely known as the Hebb learning law.

The perceptron network developed by Rosenblatt (1958) was a landmark event which initiated the engineering application of artificial neural networks.

Adaptive linear element (Adaline), a variant of perceptron, was subsequently proposed by Widrow and Hoff in 1960 and used in signaling analysis and radar antenna control. Widrow–Hoff learning law is being used in various neural network models.

At the late period of this phase, the researches on neural networks entered a recession period because of the limitation of computing ability.

(2) **Transition phase.** The key to promote the development of artificial neural networks is to propose new models and new learning algorithms, while mathematical principles of artificial neural networks are also indispensable. During the 1970s various network models, theories and learning algorithms were further proposed.

In this phase Grossberg combined psychology and brain science to form a unified artificial neural theory.

Since 1971 the Japanese scientist Amari developed some theories on dynamics and stability of artificial neural networks, in particular the theories based on manifold and probability theory.

In 1970 and 1973 Fukushima proposed the theory of neural cognitive network based on his previous researches on artificial system model of human brain. Fukushima's models include artificial neural cognition and the cognition with optional attention based on neural cognizer.

Researches on association memory made a great achievement during this period. Various association memory models were developed by Kohonen (1972), Anderson (1968, 1973, 1977), and other researchers.

(3) **Peak phase.** Since 1980, Feldman and Ballard began their neural network researches and developed various neural network systems and theories covering natural language, logistic reasoning, concept representation, parallel distributed processing, etc.

In 1982 and 1984 Hopfield published two papers on a new model and led neural network researches to the climax. Hopfield network is an interconnected and nonlinear dynamic network.

Sejnowski started his neural network researches since 1976, and proposed Boltzmann machine according to the methods and concepts of statistical physics, together with Hinton and Ackley in 1984 and 1985.

During this period a milestone algorithm for multilayer neural networks, backpropagation (BP) algorithm, was proposed by McClelland and Rumelhart in 1986.

(4) **Phase of rapid development.** The establishment of International Neural Network Society in 1987 marked the beginning of a new era of neural network researches and applications. Since then annual meetings or symposiums on neural networks have been convened around the world. Neural networks have been used in various areas of our society.

2.2. *Fundamentals of artificial neural networks*

2.2.1. *Biological neurons and mechanisms*

A typical biological neuron is composed of four parts (Bian and Zhang, 2000; Fig. 1)

(1) **Soma.** It is the body of a neuron cell. There are nucleus and cytoplast in the soma.
(2) **Dendrite.** A dendrite is typically less than 1 mm long. It receives signals from other neurons. There are thousands of branched dendrites on the soma.
(3) **Neurite.** It outputs signals to other neurons. Signals are transmitted in the neurite with the rate of dozens of meters per second. A neurite may have several branches connected to different neurons.
(4) **Synapse.** Synapse is a connection between two neurons. A synapse to dendrite is always stimulant which stimulates the next neuron and the synapse to soma is always inhibitive which inhibits the next neuron.

A neuron has two different states, i.e., stimulation and inhibition (Bian and Zhang, 2000). A neuron in inhibitive state receives the stimulant signal

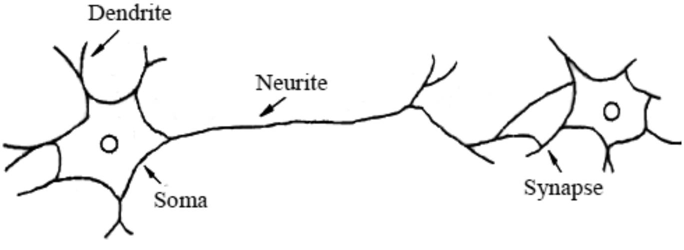

Figure 1. A biological neuron.

from other neurons. Several inputs are algebraically summed. If the sum exceeds a threshold the neuron will be inspired. It will be in a stimulant state, and delivers an output pulse to other neurons. There is a refractory period for a neuron to be inspired. This neuron will not respond to any stimulation from other neurons and the threshold will drop down gradually. Theoretically the biological neuron can only transmit Boolean signals. However, a series of pulses from a neuron when it is inspired may be treated as a frequency-modulated signal and the density of this signal may represent some continuous signal.

2.2.2. *Types and mechanisms of artificial neural networks*

A neural network can be regarded as a digraph with nodes (input nodes and neurons, or input nodes and computation nodes), synaptic connections, and functional connections. As far as connection types are concerned, there are two types of neural networks, i.e., feedforward network and feedback network. Feedforward networks are functional mapping networks and usually used for pattern recognition, function approximation and prediction (Haykin, 1994; Yan and Zhang, 2000; Fecit, 2003). Feedback neural networks are used as association memorizers and optimization tools. In a feedforward network, every neuron receives the inputs from the last layer and yields outputs for the next layer and there is not any feedback. A feedback network can be redrawn as an undigraph in which each connection is bidirectional. In a feedback neural network all nodes are computation nodes, and each node has $(n-1)$ inputs and one output if the total number of nodes is n.

There are two phases in the workflow of a neural network:

(1) **Learning phase.** The states of all computation nodes are constant and the connection weights can be adjusted through learning process.
(2) **Working phase.** Connection weights are constant during this phase and the states of computation nodes change to achieve stable states.

2.2.3. *Basic architecture of artificial neural networks*

(1) One-input neuron

The architecture of a one-input neuron is indicated in Fig. 2. The mathematical expression of the one-input neuron is

$$y = f(wx + b),$$

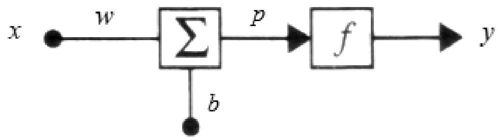

Figure 2. One-input neuron.

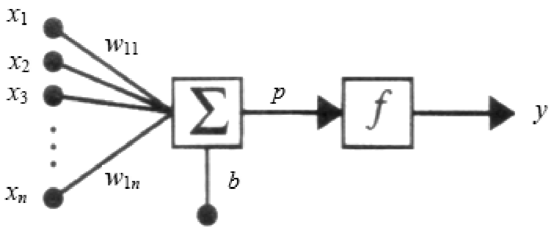

Figure 3. Multiple-input neuron. There are n inputs for the neuron.

where w = the weight of input x; b = bias; y = output; f = transfer function. In this expression, the output of accumulator, $p = wx + b$, is also called net input of transfer function f. Addition of a bias, b, can increase the adaptability of neurons and neural networks.

(2) Multiple-input neuron

The architecture of a multiple-input neuron is indicated in Fig. 3. The mathematical expression of the multiple-input neuron is

$$y = f\left(\sum w_{1i}x_i + b\right),$$

where w_{1i} = the connection weight of source neuron i to target neuron 1, $i = 1, 2, \ldots, n$; b = bias; y = output; f = transfer function.

The architecture of the multiple-input neuron (n inputs) can be briefly represented by a simpler illustration, as indicated in Fig. 4.

(3) One-layer feedforward neural network

A neuron with multiple inputs is not enough to generate a neural network. In a neural network there are generally several neurons operated in parallel (Hagan *et al.*, 1996). A set of neurons operated in parallel form a layer (Fig. 5). The mathematical expression of one-layer feedforward neural networks with s neurons is

$$y = f(wx + b),$$

where $x \in R^n$, $y \in R^s$, $b \in R^s$, and $w = (w_{ij})_{s\times n}$.

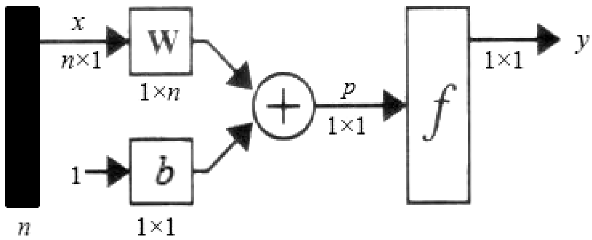

Figure 4. The simpler representation of a multiple-input neuron. In this representation x is a $n \times 1$ input vector; w is the $1 \times n$ weight vector; b, p and y are scalar constant and variables.

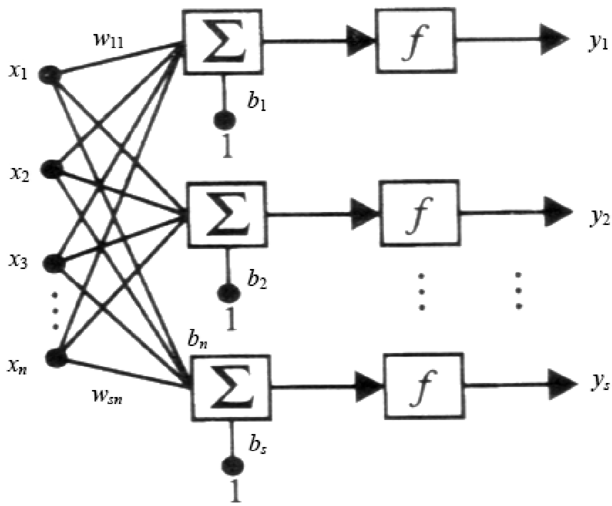

Figure 5. A one-layer feedforward network with s neurons. Each neuron has n inputs.

The architecture of one-layer feedforward networks with s neurons is briefly represented by a simpler illustration, as indicated in Fig. 6.

The number of neurons in a one-layer feedforward neural network is completely dependent on the number of network outputs.

(4) Multilayer feedforward neural network

In a multilayer feedforward neural network, each layer has its bias vector, net input vector, weight vector, and output vector. The layer with its output as the network output is output layer and the remaining layers are hidden

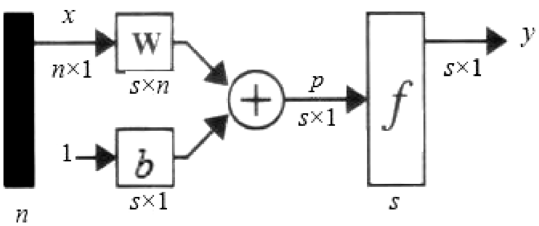

Figure 6. The simpler representation of a one-layer feedforward network with s neurons. In this representation x is $n \times 1$ input vector; w is the $s \times n$ weight matrix; b, p and y are $s \times 1$ vectors.

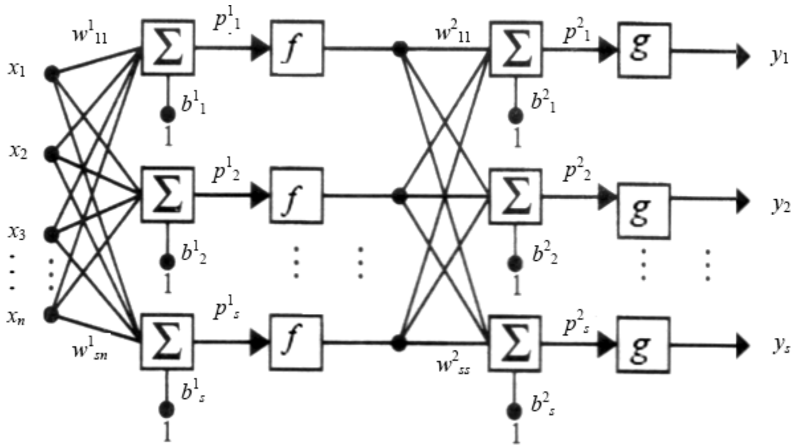

Figure 7. A two-layer feedforward neural network with s neurons in each layer. Each neuron of the first layer receives n inputs.

layers. A multilayer feedforward neural network, such as the network using sigmoid transfer function in the first layer and linear transfer function in the second layer, may arbitrarily approximate most functions (Hagan *et al.*, 1996).

A two-layer feedforward neural network, as indicated in Fig. 7, is represented by the following equation:

$$y = g(w^2 f(w^1 x + b^1) + b^2),$$

where $x \in R^n$, $y \in R^s$, $b^1 \in R^s$, $b^2 \in R^s$, $w^1 = (w^1_{ij})_{s\times n}$, and $w^2 = (w^2_{ij})_{s\times s}$.

As for the number of layers, two or three layers are enough in most cases.

There is not any reasonable algorithm or rule to determine the number of hidden neurons in a multilayer feedforward neural network.

(5) Recursive neural network

A recursive network is a feedback neural network in which some of the net outputs are redirected to inputs. Recursive networks are more powerful than feedforward networks.

A recursive network contains one or more time-delay modules that form the network feedback. The mathematical representation of a time-delay element (Fig. 8) is

$$y(t) = x(t-1),$$

where $y(0)$ is the initial condition.

Figure 9 illustrates the architecture of a recursive neural network.

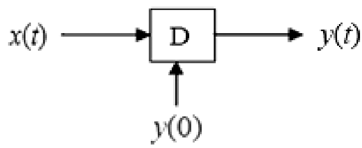

Figure 8. Time-delay element.

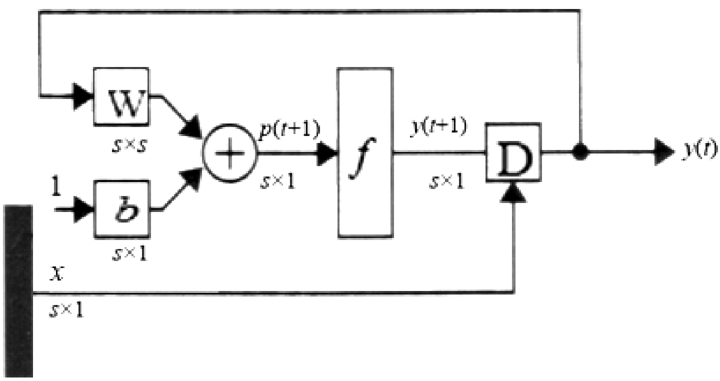

Figure 9. A recursive neural network.

2.2.4. *Learning methods of artificial neural networks*

There are three ways of network learning:

(1) **Supervised learning.** There is a set of training samples and neural network adjusts its connection weights according to the difference between given outputs and actual outputs;
(2) **Unsupervised learning.** Neural network adjusts connection weights according to statistical information carried by environmental data (Yan and Zhang, 2000), which is a self-organizing process;
(3) **Reinforcement learning.** In this learning system the external environment yields evaluation to network output and neural network adjusts its connection weights through reinforcing those actions encouraged by external environment. It is a learning method between supervised and unsupervised learning.

Three kinds of learning algorithms are used in neural networks (Yang and Zhang, 2000)

(1) **Hebb learning law.** The strength of connection between two neurons is expected to increase if the activation of the two neurons is synchronous and decrease if the activation is asynchronous, e.g., to minimize the following weight change

$$\Delta w_{ij}(t) = \eta x_i(t) y_j(t),$$

where $x_i(t)$ and $y_j(t)$ are states of two connected neurons at time t.
(2) **Error correction learning law.** The error is

$$e_i(t) = y_i(t) - z_i(t),$$

where $y_i(t)$ = desired output of ith neuron at time t; $z_i(t)$ = actual output of ith neuron at time t; $e_i(t)$ = output error of ith neuron at time t. The goal is to minimize some function of $e_i(t)$. An example is the delta rule:

$$\Delta w_{ij}(t) = \eta e_i(t) x_j(t),$$

where $x_i(t)$ is the ith input at time t, and $\Delta w_{ij}(t)$ is the weight change.

(3) **Competitive learning law.** All output nodes compete with each other and finally only the strongest node is activated. Generally there are prohibitive connections among output nodes. The learning law can be represented by the following:

$$\Delta w_{ij}(t) = \eta(x_j(t) - w_{ji}(t)), \text{ if node } j \text{ wins the competition;}$$
$$\Delta w_{ij}(t) = 0, \text{ if node } j \text{ fails in the competition.}$$

2.2.5. *Adaptation of artificial neural networks*

A neural network may ideally acquire knowledge by learning from the steady environment. However, if the environment is unsteady (time-changing), the neural network must be provided with the adaptive ability in order to follow the changing environment (Yan and Zhang, 2000). In this case every different input will be treated as a new data set and the neural network is thus viewed as a predictor:

$$x(t) = f(x(t-1), w(t-1)),$$
$$e(t) = z(t) - x(t),$$

where $z(t)$ = observed output at time t; $x(t)$ = predicted output at time t; $e(t)$ = output error at time t. The goal is to let $e(t) = 0$.

2.3. *Applications of artificial neural networks*

Neural networks are currently applied in many areas (Haykin, 1994; Widrow, 1994; Hoffmann, 1998; Zhang, 2007a–d). Some are listed below:

(1) Numerical computation. Function approximation, interpolation, optimization, etc.
(2) Modeling. Chemical modeling, ecological modeling, dynamic modeling of industrial processes, etc.
(3) Data mining and knowledge discovery. Between-variable relationship discovery, classification, etc.
(4) Biological and medical applications. Gene discovery, protein prediction, biodiversity analysis, growth simulation, survival analysis, community prediction, etc.

(5) Environmental applications. Pollutant prediction, environmental monitoring, habitat discrmination, etc.
(6) Visual and audio recognition and processing. Face and signature recognition, radar and sonic image processing (image compression, feature extraction, noise removal, etc.), robot visualization, target identification, audio compression and recognition, recognition of human tissues and cells, etc.
(7) Control systems. Robot control, orbit control, traffic dispatch and control, production flow control, weapon manipulation, target tracking, etc.
(8) Diagnostic systems. Disease diagnosis, vehicle diagnosis, machine and flow diagnosis, cardiograph classification, etc.
(9) Industry and manufacturing. Quality monitoring and analysis, performance analysis, project bidding, product design and analysis, oil exploration, etc.
(10) Communication systems. Route selection, aero-navigation, echo canceling, etc.
(11) Economic and financial applications. Market analysis, advisory system of stock exchange, real estate assessment, loan consultation, financial analysis, price prediction, cheque recognition and cash detection, etc.

2.4. *Ecological applications of artificial neural networks*

Since the 1970s ecologists have been able to understand the ecosystems by constructing mechanistic models. However, as the complexity of ecosystems studied increased, more and more black boxes emerged in the model and model complexity increased rapidly. The effectiveness and validity of mechanistic models declined at the increase of model complexity. Those models finally became unsolvable, unstable, and unreliable. Due to the complexity of ecosystems, empirical models regained popularity in recent years (Tan *et al.*, 2006). On the other hand, ecological relationships are highly nonlinear and thus could not be reasonably described by classical models (Schultz and Wieland, 1997; Pastor-Barcenas *et al.*, 2005), including both mechanistic and empirical models.

Artificial neural networks have been recognized as the universal function approximators for complex and nonlinear ecological relationships

(Acharya *et al.*, 2006; Nour *et al.*, 2006; Zhang and Barrion, 2006; Zhang, 2007a–d; Zhang *et al.*, 2008). They have the advantages of more automated model synthesis and analytical input–output models (Tan *et al.*, 2006). A large number of studies on ecological applications of artificial neural networks were conducted in the last ten years.

Concerning the dynamic modeling of ecological or environmental processes, artificial neural networks were used for modeling short and middle long-term concentration levels (Viotti *et al.*, 2002), subsurface process (Almasri and Kaluarachchi, 2005), sediment transfer (Abrahart and White, 2001), subsurface drain outflow and nitrate–nitrogen concentration in tile effluent and surface ozone (Sharma *et al.*, 2003; Pastor-Barcenas *et al.*, 2005), flow and phosphorus concentration (Nour *et al.*, 2006), dioxide dispersion (Nagendra and Khare, 2006), the growth of Chinese cabbage (Zhang *et al.*, 2007), and food intake dynamics of a holometabolous insect (Zhang *et al.*, 2008).

Artificial neural networks are always used to make classification, recognition, and prediction of ecological issues. They were used to explain the observed structure of functional feeding groups of aquatic macroinvertebrates (Jorgensen *et al.*, 2002). Backpropagation (BP) and radial basis function (RBF) neural networks were used to simulate and predict species richness of rice arthropods (Zhang and Barrion, 2006). They were used in the classification and discrimination of vegetation (Marchant and Onyango, 2003; Filippi and Jensen, 2006), habitat zones and functional groups of invertebrates (Zhang, 2007c,d). In addition, artificial neural networks have been used to explain observed changes in species composition and abundance (Jaarsma *et al.*, 2007), to construct transfer functions that implement organism–environment relationships for paleoecological uses (Racca *et al.*, 2007), to classify community assemblages (Zhang, 2007c,d; Tison *et al.*, 2007), and to determine the risk of insect pest invasion (Watts and Worner, 2009).

Spatial distribution patterns of invertebrates can be effectively described by artificial neural networks (Cereghino *et al.*, 2001; Zhang *et al.*, 2008). They performed better than partial differential equation and spline function.

Artificial neural networks have been compared to various conventional models in terms of modeling performance. They were proved to be more effective than differential equations (Zhang *et al.*, 2007; Zhang and Wei, 2009). They were superior to linear models, generalized additive models, and regression trees (Moisen and Frescino, 2002). They outperformed logistic regression, multiple discriminant model and multiple regression in predicting community composition (Olden *et al.*, 2006) and the number of salmonids (McKenna, 2005). They can also provide a feasible alternative to more classical spatial statistical techniques (Pearson *et al.*, 2002).

The need for better techniques, tools and practices to analyze ecological systems within an integrated framework has never been so great (Shanmuganathan *et al.*, 2006). Approaches conditioned on data should thus be preferred. Artificial neural networks are universal and adaptive data-driven models. Wider ecological application of them is expected in the future.

2.5. *Important books and journals*

There are a large number of books and journals on artificial neural networks. Some books on theories and applications of artificial neural networks are as follows:

(1) Anderson JA. *An Introduction to Neural Networks.* MIT press, Cambridge, USA, 1995
(2) Smith SM. *Neural Networks for Statistical Modeling.* van Nostrand Reinhold, New York, USA, 1993
(3) Chester M. *Neural Networks*: *A Tutorial.* Prentice-Hall, New Jersy, USA, 1993
(4) Hassoun MH. *Fundamentals of Artificial Neural Networks.* MIT Press, Cambridge, USA, 1995
(5) Kohonen T. *Self-Organizing Maps.* Springer-Verlag, Germany, 1995
(6) Haykin S. *Neural Networks*: *A Comprehensive Foundation.* Macmillan, New York, USA, 1994
(7) Nigrin A. *Neural Networks for Pattern Recognition.* MIT Press, Cambridge, USA, 1993
(8) Fecit. *Analysis and Design of Neural Networks in MATLAB 6.5.* Electronics Industry Press, Beijing, China, 2003
(9) Hagan MT, Demuth HB, Beale MH. *Neural Network Design.* PWS Publishing Company, Boston, USA, 1996

(10) Yan PF, Zhang CS. *Artificial neural networks and simulated evolution.* Tsinghua University Press, Beijing, China, 2000
(11) Zhang WJ. *Methodology on Ecology Research.* Sun Yat-Sen University Press, Guangzhou, China, 2007

Some journals on theories and applications of artificial neural networks are listed below:

(1) *Neural Networks*
http://www.elsevier.com/locate/neunet
(2) *Neural Computation*
http://www.mitpressjournals.org/loi/neco
(3) *Artificial Intelligence*
http://www.elsevier.com/locate/artint
(4) *IEEE Transactions on Neural Networks*
(5) *Journal of Artificial Neural Networks*
(6) *Machine Learning*
http://www.springerlink.com/content/100309/
(7) *Network*: *Computation in Neural Systems*
http://www.informaworld.com/smpp/title~db=all~content=t713663148
(8) *International Journal of Neural Systems*
http://www.worldscinet.com/ijns/ijns.shtml
(9) *IEEE Transactions on Circuits and Systems*
(10) *Ecological Modeling*
http://www.elsevier.com/locate/ecolmodel
(11) *Ecological Complexity*
http://www.elsevier.com/locate/ecocom