PAPER

An Analysis on Additive Effects of Nonlinear Dynamics for Combinatorial Optimization

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SUMMARY We analyze additive effects of nonlinear dynamics for combinatorial optimization. We apply chaotic time series as noise sequence to neural networks for 10-city and 20-city traveling salesman problems and compare the performance with stochastic processes, such as Gaussian random numbers, uniform random numbers, $1/f^{\alpha}$ noise and surrogate data sets which preserve several statistics of the original chaotic data. In result, it is shown that not only chaotic noise but also surrogates with similar autocorrelation as chaotic noise exhibit high solving abilities. It is also suggested that since temporal structure of chaotic noise characterized by autocorrelation affects abilities for combinatorial optimization problems, effects of chaotic sequence as additive noise for escaping from undesirable local minima in case of solving combinatorial optimization problems can be replaced by stochastic noise with similar autocorrelation.

key words: chaos, neural networks, combinatorial optimization problems, traveling salesman problems, surrogation

1. Introduction

Recently, novel approach with neural dynamics for combinatorial optimization problems has been discussed. The basic framework of this approach was formulated by Hopfield and Tank[1]–[3]. They applied recurrent neural networks with a kind of gradient descent dynamics decreasing computational energy function to the traveling salesman problems (TSP). Although this approach was very attractive from the viewpoint of applications of artificial neural networks, it is well known that the Hopfield neural network has a serious problem; namely, the energy function has many undesirable local minima at which neural network dynamics gets stuck due to the simple gradient descent dynamics.

In order to overcome such a problem, new methods with chaotic dynamics have been proposed [4]—[12]. These researches are qualitatively classified into two methods; the first is based upon chaotic neural networks composed of neuron models with chaotic dynamics [13], [14], and the second simply introduces chaotic sequence to each neuron as additive noise.

The first approach is based upon spatio-temporal dynamics of the chaotic neural networks [13], [14],

Manuscript received March 1, 1996.

Manuscript revised June 10, 1996.

which makes it possible for neural networks to escape from local minima of the simple gradient descent neurodynamics. Nozawa modified the Hopfield-Tank neural network by the Euler's method to a neural network possessing negative self-feedback connections, which is equivalent to the chaotic neural network [13], [14], and applied it to the TSP[4],[6]. Yamada et al. investigated the solving ability of the TSP with chaotic neural networks by comparing it with that of a stochastic neural network model. They suggested that chaotic dynamics is more effective for solving combinatorial optimization problems such as the TSP than the stochastic neurodynamics [5]. They also implied that dynamics of chaotic neural networks near "an edge of chaos [15], [16]," has higher solving abilities [7]. The effectiveness of chaotic simulated annealing was also shown by Chen and Aihara with applications to the TSP and maintenance scheduling problems in a power system [8], [9]. An advantage of chaotic simulated annealing is implied by comparing with the conventional stochastic simulated annealing. Hasegawa et al. also applied chaotic neurodynamics to the TSP. They constructed chaotic neural networks with two internal states and showed its potential abilities for solving combinatorial optimization problems such as the TSP[10].

On the other hand, in the second approach, chaotic dynamics are used as additive noise for escaping from undesirable local minima [11], [12]. Hayakawa and Sawada applied chaotic noise to the local minimum problem of the Hopfield neural network and showed that chaotic noise is more effective than stochastic noise. They implied that a kind of short time correlation of chaotic noise may be relevant to the ability for combinatorial optimization [11]. Onodera et al. also showed effects of external noise to the Hopfield neural network [12] by applying filtered chaotic sequence with finite response filters to a 6-city TSP. They investigated the effects of chaotic noise by changing autocorrelation of the noise, and implied that correlated noise is effective for the combinatorial optimization.

In this paper, we analyze the additive effects of chaotic dynamics for combinatorial optimization problems of 10-city and 20-city TSPs. We apply chaotic noise [11] to a neural network for solving the TSP and compare its performance with stochastic noise. As

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stochastic noise, white noise, colored noise with $1/f^{\alpha}$ spectra and surrogate noise [17] are introduced. Surrogate noise is a kind of stochastic time series which preserves statistical properties of the chaotic time series [17]. With such stochastic time series, we can investigate what kinds of statistical features are influential in solving combinatorial optimization problems with the neural network dynamics.

2. Solving Traveling Salesman Problems with Neural Networks

The method for solving the TSP with computational energy function of a neural network was originally proposed by Hopfield and Tank [3]. They showed that the state of the neural network converges to a stable equilibrium point corresponding to a local minimum of the energy function. We fundamentally adopt this formulation for the TSP[3]. Namely, in order to solve the TSP with N cities, $N \times N$ neurons are arranged on the $N \times N$ grid. The firing of the (i,j)th neuron means that a city i is visited on the j th order. The following energy function is defined for the neural networks [3],

$$E_{tsp} = A \left[\left\{ \sum_{i=1}^{N} \left(\sum_{k=1}^{N} x_{ik}(t) - 1 \right)^{2} \right\} + \left\{ \sum_{k=1}^{N} \left(\sum_{i=1}^{N} x_{ik}(t) - 1 \right)^{2} \right\} \right] + B \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{k=1}^{N} d_{ij} x_{ik}(t) \left\{ x_{jk+1}(t) + x_{jk-1}(t) \right\},$$

$$(1)$$

where A and B are positive constants, d_{ij} is the distance between the cities i and j. From Eq. (1), the synaptic connection weight between the (i,k) th neuron and the (j,l) th neuron and the threshold of the (i,k) th neuron are defined as follows,

$$w_{ikjl} = -A\{\delta_{ij}(1 - \delta_{kl}) + \delta_{kl}(1 - \delta_{ij})\} - Bd_{ij}(\delta_{lk+1} + \delta_{lk-1}),$$
(2)

$$\theta_{ik} = 2A,\tag{3}$$

where δ_{ij} denotes the Kronecker's delta and all of self connections are assumed to be 0.

When the noise or chaotic dynamics is injected to the neural networks described above, the state keeps wondering and never converges. Therefore, it is important how we observe the outputs of the networks. In order to obtain high solving abilities, the following observation is used in Ref. [4]-[7]. In this paper, we also introduce such observation, namely $x_{ik}(t)$ is replaced by $\bar{x}_{ik}(t)$ which is an average firing rate of short term τ

between $t - \tau + 1$ and t defined as follows:

$$\bar{x}_{ik}(t) = \frac{1}{\tau} \sum_{l=t-\tau+1}^{t} x_{ik}(l),$$
 (4)

where, in this paper, the average time $\tau=20$ which is the same value of τ used in [4]-[7]. In order to obtain an alternative output value of 0 or 1, we define firing and resting of the (i,j)th neuron at time t by following $\hat{x}_{ij}(t)$:

$$\hat{x}_{ij}(t) = \begin{cases} 1, & \text{if } \bar{x}_{ij}(t) \ge \tilde{x}(t), \\ 0, & \text{otherwise,} \end{cases}$$
 (5)

where "1" and "0" denote firing and resting of neurons respectively, and $\tilde{x}(t)$ is the N th largest value of $\bar{x}_{ij}(t)$ [4].

3. Performance Evaluation of Solving the TSP by Chaotic Noise

3.1 Chaotic Noise and White Noise

In this paper, we study the effects of chaotic noise for solving combinatorial optimization problems. On the basis of a discrete-time neural network with symmetric connections [1]-[3], we analyze the effects of additive chaotic noise by comparing with those of stochastic noise [11]. We define the dynamics of each neuron as follows:

$$x_{ik}(t+1) = f \left[\sum_{j=1}^{N} \sum_{l=1}^{N} w_{ikjl} x_{jl}(t) + \theta_{ik} + \beta z_{ik}(t) \right],$$
(6)

where f is sigmoidal function, $f(z) = 1/(1 + \exp(-z/\epsilon))$, $\epsilon = 0.3$, $z_{ik}(t)$ is an added noise sequence for the (i,k)th neuron, which is normalized to zero mean and unit variance, and β is a scaling constant. In this neural network model, chaos is injected to the each neuron dynamics as additive noise. In this paper, we analyze such additive effects of chaotic noise for combinatorial optimization. Here we adopt the logistic map as an example of chaotic noise, which is described as follows:

$$z_{ik}(t+1) = rz_{ik}(t)(1 - z_{ik}(t)), \tag{7}$$

where r is a bifurcation parameter. Since the logistic map is the most familiar discrete map with chaotic dynamics, it is introduced in the first experiment. First of all, we introduce uniformly distributed random numbers and Gaussian distributed random numbers, as stochastic noise. Solving abilities by chaotic noise from the logistic map with r=3.95, the uniformly distributed noise and the Gaussian noise for the TSP are shown in Table 1. Table 1 shows the result of 10-city and 20-city TSPs shown in Figs. 1 and 2. In this paper,

Table 1 Solving abilities (%)in case of adding chaotic noise and stochastic noise for the 10-city (in Fig. 1) and 20-city traveling salesman problems (in Fig. 2).

The number of cities		20
chaotic noise (logistic map; $r = 3.95$)	100	94
uniformly distributed random noise	87	1
Gaussian distributed random noise	88	0

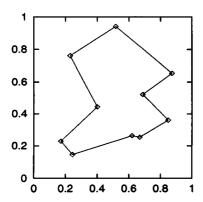


Fig. 1 A 10-city traveling salesman problem by Hopfield and Tank [3]. Diamonds (⋄) indicate cities, and solid lines indicate the optimum solution.

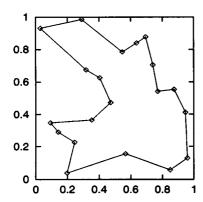


Fig. 2 A 20-city traveling salesman problem. Diamonds (♦) indicate cities, and solid lines indicate the optimum solution.

the solving ability is defined as the rate that the network finds an optimum solution among 100 different initial conditions. Here it is defined that the network finds an optimum solution if the state of neural network hits an optimum solution at least once within 1,000 iterations. In this paper, we use 100 different initial states for each experiment in order to average dependence on the initial states. In this experiment, $A=1, B=1, \beta=0.35$. In Table 1, chaotic noise shows the best solving ability. Similar results can be obtained with other values of parameter β , such as $\beta=0.3$. Therefore, in the following subsections, we analyze the effects of chaotic noise by comparing with other kinds of stochastic noise, such as $1/f^{\alpha}$ -type noise and surrogate noise [17].

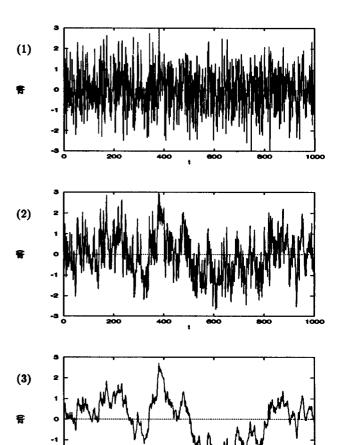


Fig. 3 Time series of $1/f^{\alpha}$ noise, in case of (1) $\alpha=0.0$ (corresponding to white noise), (2) $\alpha=1.0$ and (3) $\alpha=2.0$.

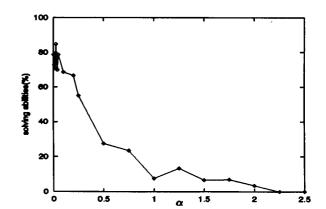


Fig. 4 Solving abilities on a 10-city TSP[3] by using $1/f^{\alpha}$ noise in case of changing α .

3.2 $1/f^{\alpha}$ -Type Noise

Examples of time series of $1/f^{\alpha}$ noise are shown in Fig. 3. By changing the value of α , various $1/f^{\alpha}$ -type stochastic time series with different autocorrelation can be realized.

Solving abilities of $1/f^{\alpha}$ noise, with $A=1,\,B=1$

and $\beta=0.35$, are shown in Fig. 4, in case of changing α . Figure 4 shows that smaller values of α have higher solving abilities. It implies that autocorrelation should be low for effective combinatorial optimization in this situation. However, from Table I, chaotic noise exhibits better on solving abilities than white noise which corresponds to $\alpha=0$, or the lowest autocorrelation in Fig. 4. From these results, it is suggested that properties peculiar to chaotic noise, for example, autocorrelation function shown in Fig. 6, may provide good effects for solving combinatorial optimization problems. Therefore, we investigate solving abilities of chaotic noise with the method of surrogate data, which can preserve statical properties, such as autocorrelation function.

3.3 Surrogate Noise[17]

Then, we analyze what kinds of properties influence solving abilities for combinatorial optimization on the basis of surrogate data sets [17].

The method of surrogate data is usually introduced to obtain reliable results in the field of nonlinear time series analysis [18], [19]. It is well understood that careless estimation of nonlinear statistics such as fractal dimension, or Lyapunov exponents [18], [19], [21] could lead to spurious identification of existence of chaos underlying time series data. In chaotic time series analysis, in order to avoid such spurious estimates of nonlinear statistics evaluating chaotic dynamics, a null hypothesis with some linear stochastic process to the observed time series is introduced and checked whether or not it can be rejected on the basis of surrogate data sets generated according to the null hypothesis [17].

In this paper, we utilize a different aspect of the method of surrogate data; namely, surrogates can preserve several statistics of the original time series, such as, empirical histograms and autocorrelation [18]. For example, if the observed time series is hypothesized to be characterized only by linear process, for example, AR model, then the time series can be characterized by autocorrelation.

In this paper, we use the method of surrogate data for controlling preservation of statistics of the original data; four algorithms for making surrogate data sets are introduced.

- Random-shuffled surrogate: The first surrogate data are made by random shuffling of the original time series. This surrogate does not preserve autocorrelation of the original data but preserves the empirical histogram.
- 2. Phase randomized (Fourier transformed) surrogate: The second surrogate data are made by the following procedure. First, the Fourier transform of the original data is calculated to obtain the power spectrum. Then the phase structure of the power spectrum is randomized. Finally the inverse

Fourier transform is calculated. The obtained surrogate data has the identical power spectrum with the original data, but do not preserve the empirical histogram.

- 3. Gaussian scaled (Amplitude adjusted Fourier transformed) surrogate: The third surrogate is made by the following procedure. First, Gaussian distributed random numbers are produced and arranged to have the same rank order as the original time series. Then, the phase randomized surrogate algorithm is executed on the rank-ordered Gaussian data. Finally, the Gaussian scaled surrogate data are obtained by shuffling the original time series so as to keep the same rank order with the obtained phase randomized surrogate data of the rank-ordered Gaussian data. The obtained surrogate preserves exactly the empirical histogram and approximately autocorrelation of the original data.
- 4. Fourier shuffled surrogate [20]: First, phase randomized surrogate data are made by the second algorithm. Then the original time series are shuffled to keep the same rank order with the obtained phase randomized data. This surrogate preserves an approximate autocorrelation and the exact empirical histogram.

The time series of the original chaotic noise from a logistic map (r=3.95) and its surrogate data sets of each algorithm are demonstrated in Fig. 5. The autocorrelation functions of each time series are shown in Fig. 6. It is clearly seen that autocorrelation of the phase randomized surrogate is exactly same as the original, and that those of Gaussian scaled and Fourier shuffled surrogates are almost same. The random shuffled surrogate data has quite different autocorrelation from the original time series. In Table 2, summarized are which statistics of each surrogate are preserved. For more detail discussions on a surrogate data set and its statistics, see Ref. [18].

Then 10-city (Fig. 1) and 20-city (Fig. 2) TSPs are solved by using a logistic map and its surrogates as additive noise in Eq. (6). The results are shown in Fig. 7 with A=1, B=1 and $\beta=0.35$ and changing the value of the parameter r. Figure 7 shows that the random shuffled surrogates have quite different solving abilities from those of the original data but the phase

Table 2 Statistics of surrogate data. \bigcirc , \triangle , \square , and \times mean preserving each statistics completely, approximately, partly and hardly, respectively [18].

	first order statistics	second order statistics
Random shuffled	0	×
Phase randomized		0
Gaussian scaled	0	Δ
Fourier shuffled		Δ

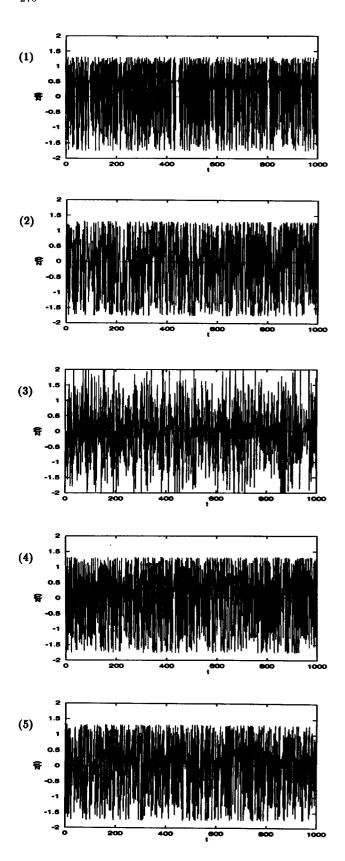


Fig. 5 Time series of the original chaotic noise (logistic map, r=3.95) and its surrogates. (1) the original time series, (2) Random shuffled surrogate, (3) Phase randomized surrogate, (4) Gaussian scaled surrogate and (5) Fourier shuffled surrogate.

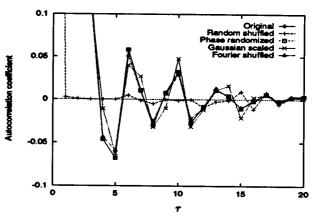


Fig. 6 Autocorrelation functions of a logistic map (r = 3.95) and its surrogate data. The length of time series is 32, 768.

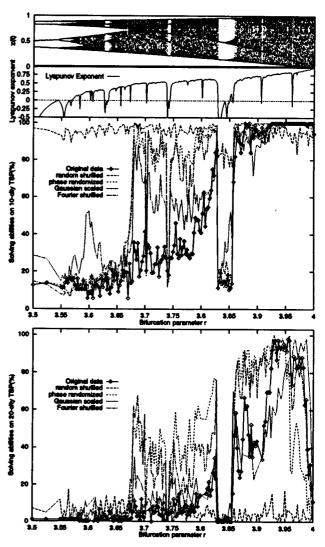


Fig. 7 Solving abilities of 10-city and 20-city traveling salesman problems with a logistic map and its surrogates. The upper figure shows a bifurcation diagram of a logistic map, and the middle figure shows Lyapunov exponents with changing the value of the parameter r.

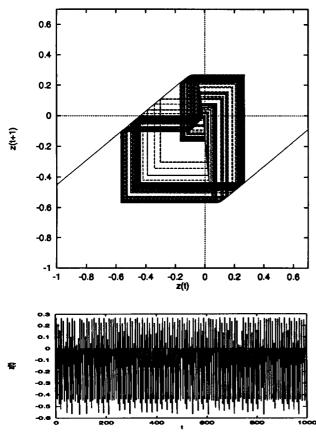


Fig. 8 Dynamics of the chaotic neuron model. The upper figure shows a return map of chaotic neuron model and the lower figure shows time series of chaotic neuron model.

randomized, Gaussian scaled and Fourier shuffled surrogates, which preserve autocorrelation exactly or approximately, have similar abilities to the original data. It suggests that temporal structure characterized by autocorrelation effects solving abilities for combinatorial optimization by chaotic noise. High solving abilities of surrogate data sets suggest that effects of chaotic sequence for solving optimization problems can be replaced by stochastic noise with similar autocorrelation.

Then, we also introduce another kind of chaotic data. Figure 9 shows the results in case of using chaotic noise from a chaotic neuron model [13], [14], which is defined by the following equation,

$$z_{ik}(t+1) = kz_{ik}(t) - \alpha f(z_{ik}(t)) + a,$$
 (8)

where f is sigmoidal function. The chaotic neuron model is a discrete bimodal map which dynamics is demonstrated in Fig. 8. In Fig. 9, the following parameter values are used: $k=0.8, \alpha=1.0$, and a is used as a bifurcation parameter. This result is obtained with A=1, B=1 and $\beta=0.35$. Figure 9 shows similar results with those of the logistic map.

In result, we could conjecture as follows: abilities of chaotic sequence as additive noise in order to solve combinatorial optimization problems can be replaced

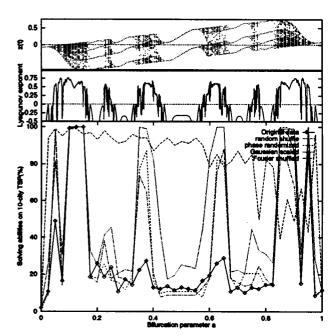


Fig. 9 Solving abilities of a 10-city traveling salesman problem with a chaotic neuron model and its surrogates. The upper figure shows the bifurcation diagram of a chaotic neuron model, and the middle figure shows Lyapunov exponents with changing the value of the parameter a.

by surrogate data sets which preserve autocorrelation of the original data.

In this paper, we introduced chaotic sequence only as memoryless additive noise to the neural network dynamics. In case of using such a method, since there are no feedback from the searching information for optimum solution; namely there is no relation between the network dynamics and state space that has been already searched. On the other hand, chaotic neural networks [13], [14] can have memory effects in each neuron dynamics. The state of chaotic neural networks depends upon the past history of the previous states of the neural network. However, dynamics of chaotic neural networks is not always effective; our previous research showed that a chaotic neural network with weak chaotic behavior has higher solving abilities than that with periodic behavior for combinatorial optimization problems (in Ref. [10]). Therefore, neural networks with only memory effects of the past history of previous states are not enough for combinatorial optimization problems, but those with chaotic behavior influence solving abilities. Then, it is suggested that chaotic neural networks have effects for combinatorial optimization not only in its chaotic dynamics but also in memory effects, so they must be more effective than an approach of using chaotic sequence as additive noise.

4. Conclusion

In this paper, we analyzed additive effects of chaotic dy-

namics for combinatorial optimization problems. We introduced chaotic sequence as additive noise source and compared the performance of the original data with stochastic time series such as Gaussian random numbers, uniform random numbers, colored noise with $1/f^{\alpha}$ spectra and surrogate data sets. In this experiment, we confirmed the previous result that chaotic noise of the logistic map is effective for the combinatorial optimization. Moreover, it is clarified that phase randomized, Gaussian scaled and Fourier shuffled surrogates have similar abilities with the original logistic map. Since these surrogates preserve the autocorrelation of the original data, it implies that solving abilities of chaotic noise is depending on its autocorrelation. Furthermore, since surrogate data sets also exhibit high solving abilities, it is suggested that effects of chaos as additive noise can be replaced with such stochastic surrogate data.

In this paper, we introduce only the first and the second order statistics, and do not discuss about higher order statistics. It is important future works to investigate solving abilities by such higher order surrogates.

On the other hand, it has already been indicated that the chaotic neurodynamics have good effects for combinatorial optimization problems [4]–[10]. It is also a future problem to investigate effects of chaotic dynamics in more detail and apply such chaotic neurodynamics to other and larger scale combinatorial optimization problems.

Acknowledgement

The authors would like to thank T. Yamada (Aihara Electrical Engineering Co., Ltd.) for fruitful discussions.

This research was partly supported by Grant-in-Aids for Scientific Research (C) to TI (No. 078321019) and for Priority Area to KA (No.08279103) from the Ministry of Education, Culture and Science of Japan.

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