Characterizing the dynamics of constrained physical systems with an unsupervised neural network

Christopher Monterola and Caesar Saloma*

National Institute of Physics, University of the Philippines, Diliman 1101, Quezon City, The Philippines

(Received 10 March 1997; revised manuscript received 10 October 1997)

The method of Lagrange multipliers is utilized in the unsupervised training of a three-layer, single-output, feed-forward neural network for characterizing the dynamics of constrained physical systems. Training aims at minimizing the energy function that is obtained from the equations of state which are generated using the method of Lagrange multipliers. The approach is illustrated (1) to solve an inverse problem in nuclear reactor design, (2) to determine how competing biological entities organized (cells in a tissue, *Eucalyptus* trees), and (3) to solve an ill-posed differential equation.
[S1063-651X(98)50502-8]

PACS number(s): 87.10.+e

We demonstrate a new neural network (NN) approach to characterizing the dynamics of constrained physical systems. The method of Lagrange multipliers (MLM) [1] is utilized in the unsupervised training of a single-output feed-forward NN.

An NN is trained to do a particular task by minimizing a certain quantity like the sum-of-squares error in supervised training, or the energy function in unsupervised training [2–5]. In other problems such as finding the principal components of an ensemble of images, training is aimed at maximizing the projection of the NN weight vector on the multidimension vector formed by the principal components [6]. In any manner, training is always aimed at finding, within the shortest possible time, the appropriate interconnection strengths between neurons that make the network yield a satisfactory solution to a given problem.

In this paper, an unsupervised NN is trained to describe the behavior of a constrained system, by minimizing the energy function whose form is derived from the equations of state which are generated via MLM.

The ability of MLM to produce functional relationships between the various dynamical variables, is combined with the hyperdimensional fitting capability of NN [2–5] to obtain a description of the dynamics of a constrained system. Given the set of K constraints $\{C_k(x_1,x_2,\ldots,x_M)=\kappa_k\}$ where $k=1,2,\ldots,K$; the cost function $F(x_1,x_2,\ldots,x_M)=F(x_i)$ is optimal when the Lagrange formulation

$$\frac{\partial F}{\partial x_i}+\sum_{k=1}^{K}\lambda_k\frac{\partial C_k}{\partial x_i}=0 \tag{1}$$

is satisfied, where λ_k's are the Lagrange undetermined multipliers. Equation (1) is used to generate the equations of state of a constrained system. The NN is trained to reduce the quantity on the left-hand side (LHS) of Eq. (1), to a predefined small value near zero. At the start of training the LHS value is far from zero, and Eq. (1) is not satisfied.

Figure 1 shows the architecture of the three-layer, feed-forward NN that is trained to output an accurate approximation of $F(x_i)$ corresponding to specific values of $x_1,x_2,\ldots,x_M$, $\lambda_1,\ldots,$ and λ_k.

The output $y_h^{\rm hi}$ of the hth hidden neuron is: $y_h^{\rm hi}=\phi_h(W_{hr}^{\rm in}y_r^{\rm in})=\sum_r[\sin(W_{hr}^{\rm in}y_r^{\rm in})+\cos(W_{hr}^{\rm in}y_r^{\rm in})]$, where $\phi_h(W_{hr}^{\rm in}y_r^{\rm in})$ is its activation function, $W_{hr}^{\rm in}$ is the connection strength between the hth hidden neuron and the rth input neuron, $y_r^{\rm in}$ is the output of the rth input neuron, $h=1,2,\ldots,D$; and $r=1,2,\ldots,(M+K+1)$. The input neurons exhibit a linear response so that $\{y_r^{\rm in}\}=(x_1,x_2,\ldots,x_M,\lambda_1,\ldots,\lambda_K,\text{bias})=\{x_1;\lambda_k,\text{bias}\}$. The NN output is: $Z_{\rm out}=\sigma(W_h^{\rm hi}y_h^{\rm hi})=\Sigma_h C_h W_h^{\rm hi}y_h^{\rm hi}$, where $\sigma(W_h^{\rm hi}y_h^{\rm hi})$ is the activation function of the output neuron, $W_h^{\rm hi}$ is the connection strength between the output neuron and the hth hidden neuron, and C_h is a multiplicative constant.

The sinusoid combination is utilized for $\phi_h(W_{hr}^{\rm in}y_r^{\rm in})$ because it permits efficient higher-order polynomial curve fitting and faster trainability [6–8]. We found, however, that training is not successful if a purely (even) cosine function is used for $\phi_h(W_{hr}^{\rm in}y_r^{\rm in})$. A linear $\sigma(W_h^{\rm hi}y_h^{\rm hi})$ is selected because $Z_{\rm out}$ is expected to cover a range of possible values. A sigmoidal output response is most suitable in pattern classification networks whose outputs operate on thresholding [6].

The final values of the interconnection strengths are determined using the gradient-descent backpropagation method

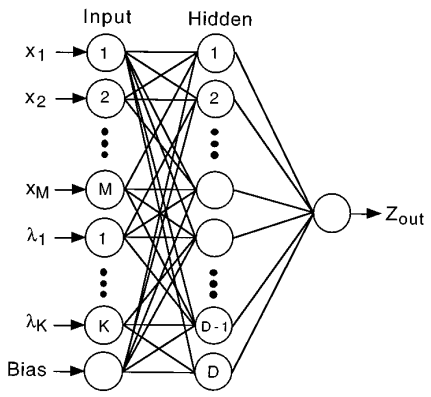

FIG. 1. Feed-forward NN for characterizing the dynamics of constrained systems. It has $(M+K+1)$ inputs, D hidden neurons, and one output.

*Electronic address: csaloma@nip.upd.edu.ph

(momentum term=0) [2–5]. The NN undergoes unsupervised training to reduce the energy function $E(y_r^{\text{in}})$ to a desired value. The strengths are updated according to: $W_{mn}^{(p+1)} = -\alpha[\partial E^{(p)}(y_r^{\text{in}})/\partial W_{mn}^{(p)}] + W_{mn}^{(p)}$, where α is the learning rate, and $W_{mn}^{(p)}$ is the previous strength value between the mth neuron in the current layer and the nth neuron in the next layer.

The training set consists of T combinations of x_i's and λ_k's values and the initial $W_{\min}$ values are chosen randomly between -1 and $+1$. The NN input number $(M+K+1)$ depends on the problem at hand while the D value is determined by trial and error, and is chosen to yield the fastest decrease in the average energy $E_{\text{av}}^{(p)}(y_r^{\text{in}})$ with increasing iteration number p.

The functional form of $E(y_r^{\text{in}})$ depends on the problem at hand, and is derived from Eq. (1). We found that the $Z_{\text{out}}(y_r^{\text{in}})$ plot accurately approximates the $F(x_i)$ profile when $E_{\text{av}}^{(p)}(y_r^{\text{in}})$ is reduced to a value at least in the order of 10^{-2}.

The NN approach is used to determine: (1) the cost function that is minimized when designing a cylindrical nuclear reactor (CNR), (2) the nearest-neighbor distributions (NND) of biological systems with competing constituents (*Eucalyptus* trees, contiguous cells in a tissue), and (3) the solution of an ill-posed second-order differential equation (DE) that describes the dynamics of heart vibrations. The problems are chosen to highlight the various advantages of the NN approach.

A CNR design must satisfy a constraint imposed by the neutron diffusion theory [1]: $C_1(R,H) = (2.4048/R)^2 + (\pi/H)^2 = \theta^2$, where H is the reactor height, R is the radius, and θ is a constant. The forward problem concerns the determination of the R and H values that minimize the CNR volume $V(R,H) = \pi R^2 H$. The cost function $F(R,H)$ is given by $V(R,H)$ and MLM shows that $V(R,H)$ is minimized only if $H = 1.847R$.

We solve the inverse problem of determining the form of $F(R,H)$ knowing that it is a minimum when $H = 1.847R$, and that $C_1(R,H) = \theta^2$. Note that it is difficult to obtain $F(R,H)$ by directly solving the coupled DE's: $(\partial F/\partial H) + \lambda_1(\partial C_1/\partial H) = 0$, and $(\partial F/\partial R) + \lambda_1(\partial C_1/\partial R) = 0$, where $F(R,H)$ is minimum when $H = 1.847R$. Equation (1) yields $(\partial F/\partial R)\partial C_1/\partial H - (\partial F/\partial H)\partial C_1/\partial R = 0$, or $[-2(2.408)^2/R^3]\partial F/\partial R + (-2\pi^2/H^3)\partial F/\partial H = Q(R = H/1.847, H) = 0$.

The NN approach exploits the fact that $F(R,H)$ is a solution to $Q(R = H/1.847, H) = 0$. The energy function to be minimized is: $E(R,H) = Q^2(R = H/1.847, H) = [(-2(2.408)^2/R^3)(\partial Z_{\text{out}}/\partial R) - 2\pi^2/H^3(\partial Z_{\text{out}}/\partial H)]^2$. Thus, $Z_{\text{out}}(R,H)$ becomes equal to $F(R,H)$ if $E(R,H)$ is reduced to zero for all $R-H$ pairs [9].

In Fig. 2 are plots of $E_{\text{av}}^{(p)}(R_t,H_t)$ vs p where $E_{\text{av}}^{(p)} = (1/T)\Sigma_t E^{(p)}(R_t,H_t)$, $R_t = H_t/1.847$, $t = 1,2,\ldots,T = 100$. Iteration number p represents the number of times that the entire set has been fully utilized in the training. The pertinent NN has only three inputs: $R = H/1.847, H, \text{bias} = 1.0$; because $Q(R,H)$ is independent of λ_1. The training set consists of 100 $R_t - H_t$ pairs with H_t equally sampled within: $0 \leqslant H \leqslant 1$. We also found that the NN still learns the correct input-output mapping even if a pure sine function is used for $\phi_h(W_{hr}^{\text{in}} y_r^{\text{in}})$.

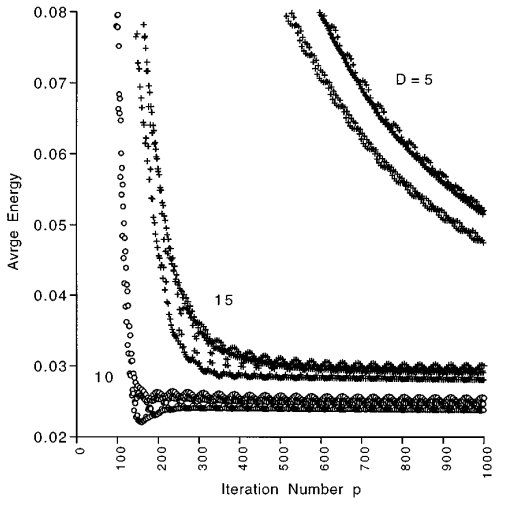

FIG. 2. CNR design. Plots of $E_{\text{av}}^{(p)}(R = H/1.847, H)$ vs iteration number p for different D values ($\alpha = 10^{-5}$, $C_h = \pi$). Choosing $C_h = \pi$ for all hidden neurons, results in faster decrease of $E_{\text{av}}^{(p)}$. Note that $E_{\text{av}}^{(1)} = 238.24$ for $D = 10$, $E_{\text{av}}^{(1)} = 431.98$ for $D = 5$, $E_{\text{av}}^{(1)} = 501.37$ for $D = 15$. Other D values ($D = 8,20,30$) were also tested but the resulting $E_{\text{av}}^{(p)}$ plots were not promising.

In Fig. 3 is the $Z_{\text{out}}(R,H)$ plot produced by a trained NN with $E_{\text{av}}^{(p)} = 0.0251$, ($p = 400$, $D = 10$). The $Z_{\text{out}}(R,H)$ plot has a normalized mean-squared error $(\text{NMSE}) = (\Sigma_m |F^T(m) - Z_{\text{out}}(m)|^2)/(\Sigma_m |F_m^T|^2) = 2.08 \times 10^{-4}$, where $Z_{\text{out}}(m) = Z_{\text{out}}(R_m, H_m)$, and $F^T(m) = V(R_m, H_m)$, and $m = 1,2,\ldots,1600$ [10]. The plot illustrates the ability of a trained NN to interpolate accurately $F(R_m, H_m)$ values corresponding to $R_m - H_m$ pairs that were not part of the training set.

We next analyze how competing biological species distributes spatially in the presence of other species. In particular, we consider (1) *Eucalyptus* trees in Queensland, Australia and (2) contiguous cells in an insect tissue. Recently [11], the principle of maximum entropy (PME) has been used to model explicitly their NND's: $\Theta(R_i) = \Theta$, where R_i is the nearest-neighbor distance of the ith individual, and $i = 1,2,\ldots,P = \text{total number of individuals in the system.}$

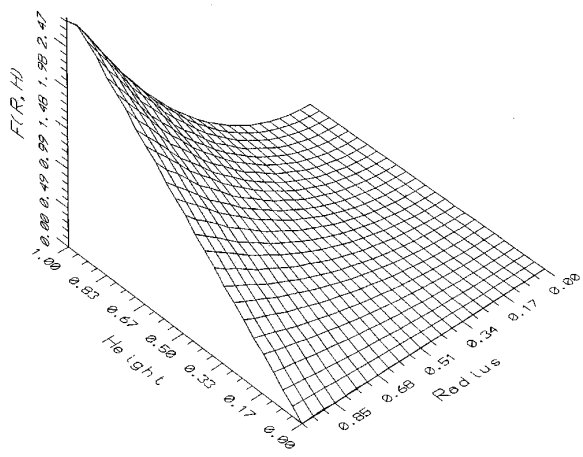

FIG. 3. CNR design. A 1600 datapoint $Z_{\text{out}}(R,H)$ plot of NN with $E_{\text{av}}^{(p)} = 0.0251$ ($D = 10$).

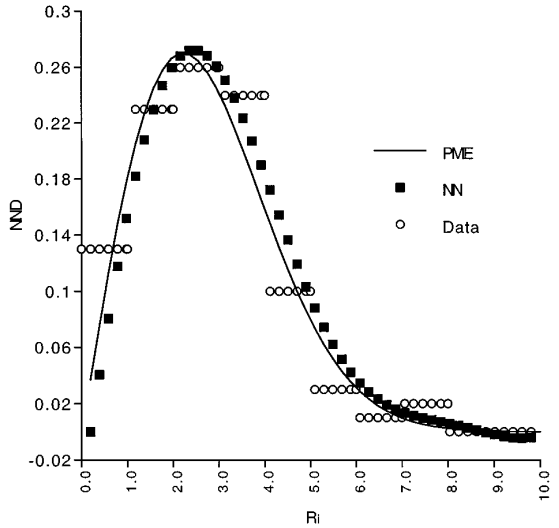

FIG. 4. NND of *Eucalyptus* trees. $Z_{\text{out}}(R_i)$ plot (squares) of NN with $E_{\text{av}}^{(p)} \approx 1.6\times10^{-2}$ ($C_h=1$, $E_{\text{av}}^{(1)} \approx 7552$). Also shown are best-fit curve $\Theta_{\text{PMB}}(R_i)$, and the experimental data plot (51 points, circles). Distance R_i is measured between the outer diameters of the trunks. The trees (average height=17 m, crown cover ranges from 6.8–10.2 m) grow in a 1000 hectare study area with another tree species, about 20 shrub species, grasses and herbs. A data point represents the NN distribution over a certain R_i range [10].

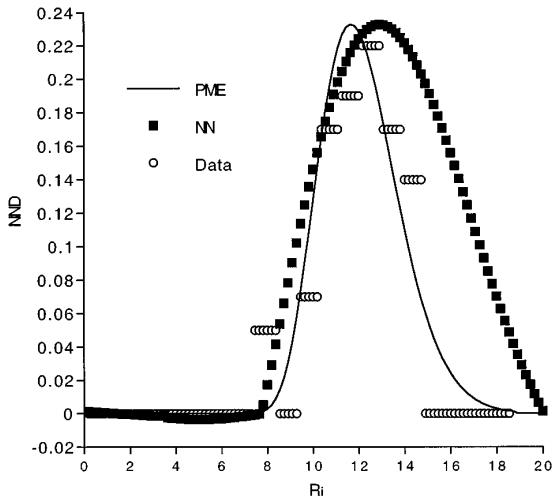

FIG. 5. NND of cells in a tissue. $Z_{\text{out}}(R_i)$ plot (squares) of NN with $E_{\text{av}} \approx 1.6\times10^{-2}$. Also shown are best-fit curve $\Theta_{\text{PME}}(R_i)$, and the experimental data (102 points, circles) where R_i (in microns) is measured between cell centers. The curves correspond to $w=12$, $\lambda_1=1.5$, and $\lambda_2=0.012$.

We used the NN approach to determine the form of $\Theta(R_i)$ using the assumption that each system behaves in a manner that maximizes its entropy $T=-k\Sigma_i[\Theta(R_i)]\log[\Theta(R_i)]$, where k is the Boltzmann constant. The dynamics are subject to the following constraints: (1) average spatial-competition pressure is constant, and (2) average nearest-neighbor area is constant.

Constraint 1 implies that the average-competition pressure of a pattern is given by: $U_0=\Sigma_i\Theta(R_i)U(R_i)=C_1=\text{const.}$ Constraint 2 implies that $A_0=\pi\Sigma_i R_i^2\Theta(R_i)=C_2=\text{const.}$ Quantities U_0 and A_0 represent the repulsive interaction between individuals, and their tendency to aggregate, respectively. The pressure $U(R_i)$ between interacting species is $U(R_i)=\exp(-R_i^2/4w^2)/[1-\exp(-R_i^2/4w^2)]$ where w is the effective size of the species. Equation (1) yields the following equation of state: $[\partial T/\partial\Theta]+\lambda_1[\partial U_0/\partial\Theta]+\lambda_2[\partial A_0/\partial\Theta]=0$. Multiplier λ_1 represents the combined effect of environmental factors (biological species, temperature, availability of resources, etc.) and λ_2 is the number density.

The pertinent NN has five inputs $(R_i, w, \lambda_1, \lambda_2, \text{bias}=0)$ and $D=15$. The energy function to be minimized is $E(R_i,w,\lambda_1,\lambda_2)=[(\partial T'/\partial Z_{\text{out}})+\lambda_1(\partial U_0'/\partial Z_{\text{out}})+\lambda_2(\partial A_0'/\partial Z_{\text{out}})]^2$, where $T'=-k\Sigma_i Z_{\text{out}}(R_i)\log[Z_{\text{out}}(R_i)]$, $U_0'=\Sigma_i Z_{\text{out}}(R_i)U(R_i)$, and $A_0'=\pi\Sigma_i R_i^2 Z_{\text{out}}(R_i)$. The training set consists of $2\times10^4 R_i-w-\lambda_1-\lambda_2$ combinations where $5<R_i<10$, $0.5<w<4$, $0.1<\lambda_1<1$, and $0.1<\lambda_2<1$.

Figure 4 shows the $Z_{\text{out}}(R_i)$ plot produced by a trained NN with $E_{\text{av}}^{(p)} \approx 1.6\times10^{-2}$ ($p=1.2\times10^4$). Also plotted is the best-fit curve $\Theta_{\text{PME}}(R_i)$ that is obtained by analytically solving the equation of state and then finding the values of w, λ_1, and λ_2 ($w=0.5m$, $\lambda_1=0.01$, and $\lambda_2=0.03$) that fit best the experimental data [11].

Within the training range $5<R_i<10$, the differences $|\Theta_{\text{PME}}(R_i)-Z_{\text{out}}(R_i)|$ are small (relative NMSE=0.3231). In the range $0.196\leqslant R_i<5$, the trained NN performs an extrapolation and the $|\Theta_{\text{PME}}(R_i)-Z_{\text{out}}(R_i)|$ values are larger. Note that (1) $Z_{\text{out}}(R_i)=0$ at $R_i=0.196$, (2) the data and $Z_{\text{out}}(R_i)$ plots have the same peak positions, and (3) $Z_{\text{out}}(R_i)$ values coordinate more closely with data within $7\leqslant R_i<8$.

To illustrate its versatility, the same trained NN is utilized to determine the NND of contiguous cells in a tissue of an adult insect [11–12]. Figure 5 shows the $Z_{\text{out}}(R_i)$ plot obtained when $w=12$, $\lambda_1=1.5$, and $\lambda_2=0.012$. Note that the peak of $Z_{\text{out}}(R_i)$ plot is located nearer to the one exhibited by the data. The results illustrate that a trained NN can be immediately employed to determine the NND's of other biological entities whose dynamics are described by the same energy function.

Our last problem emphasizes the ability of the NN approach to solve DE's. In particular, we examine the operation of a cardiograph that converts the heart vibrations into mechanical displacements. The patient rests on a horizontal tabletop which can vibrate only horizontally (along the x axis) and in response to the pumping of his heart.

The table displacement $x(t)$ satisfies: $Md^2x/dt^2+\beta dx/dt+\gamma x=F=md^2y/dt^2$, where M is the combined mass of system (patient plus moving tabletop), F is the force on the system due to the pumping action of the heart, m is the mass of blood pumped out of the heart during each vibration, y is the instantaneous location of the center of mass of m, and β and γ are proportionality constants. We assume that the system also experiences a velocity-dependent damping force, and a position-sensitive restoring force.

In general [13], the heart vibrates in a complicated manner so that $y(t)=\Sigma_m c_m \sin(2\pi m f_0 t)$, where c_m's are the Fourier series coefficients, and f_0 is the fundamental frequency. If $y(t)=c_1\sin(2\pi f_0 t)+c_2\sin(4\pi f_0 t)$, then the steady-state (particular) solution is

$$x_a(t)=[4m\pi^2 f_0^2 c_1/(4M\pi^2 f_0^2-\gamma)^2+4\beta^2\pi^2 f_0^2]$$
$$\times[(4M\pi^2 f_0^2-\gamma)\sin(2\pi f_0 t)+2\beta\pi f_0\cos(2\pi f_0 t)]$$
$$+[16m\pi^2 f_0^2 c_2/(16M\pi^2 f_0^2-\gamma)^2+16\beta^2\pi^2 f_0^2]$$
$$\times[(16M\pi^2 f_0^2-\gamma)\sin(4\pi f_0 t)+4\beta\pi f_0\cos(4\pi f_0 t)].$$

We examine if the NN approach is also capable of finding the steady-state solution in the case when $\beta>0$ where the transient (homogeneous) solution is negligible. The energy function to be minimized is: $E(t,f_0,M,\beta,\gamma)=[Md^2Z_{\text{out}}/dt^2+\beta dZ_{\text{out}}/dt+\gamma Z_{\text{out}}-md^2y/dt^2]^2$, with $c_1=c_2=1$. Note that the problem is ill-posed because two constraints are not available to provide a unique solution to the second-order DE. Traditional numerical methods can not handle ill-posed DE's [14].

The pertinent NN has six inputs ($t, w=2\pi f_0, M, \beta, \gamma$, bias$=0$) and $D=15$ ($C_h=1$). The training set consists of 1.5×10^5 t-w-M-β-γ combinations where: $0<t<3$, $0.5<w<4$, $0.01<M<0.05$, $0.5<\beta<2.5$ and $0.01<\gamma<0.05$. During training, α was occasionally varied between 10^{-2} and 10^{-5}, to force $E_{\text{av}}^{(p)}$ to decrease rapidly. Training started with $E_{\text{av}}^{(1)}\approx1663$, and was stopped at $E_{\text{av}}^{(3000)}\approx10^{-4}$.

Shown in Fig. 6 are plots of $Z_{\text{out}}(t)$ for $f_0=0.5$, 1, 2, 3, and 4 ($M=0.1$, $\beta=2$, $C_h=1$, $C_h=1$, and $\gamma=0.01$). The NMSE's of the plots relative to the corresponding analytic solutions, are all in the order of 10^{-2}. The results indicate that the trained NN generalizes very well and provides an accurate approximation of $x_a(t)$ for all t values. This particular example shows the suitability of the NN approach to problems that require the value of the solution in real time.

This paper is about an NN approach to characterizing the dynamics of constrained systems. Three widely different examples of constrained physics are investigated to illustrate the applicability of the approach. In all cases, Z_{out} provides a good fit either of the analytic solution or the real data, once the corresponding $E_{\text{av}}^{(p)}$ is reduced to a value that is at least in the order of 10^{-2}.

The efficacy of the NN approach to describing the dynamics of a given physical phenomenon, presupposes that the pertinent cost function and its constraints have been correctly identified so that the expression in the left-hand side of Eq. (1) is formulated correctly. An accurate description of the system dynamics will be impossible to obtain if the NN is trained using an erroneous energy function.

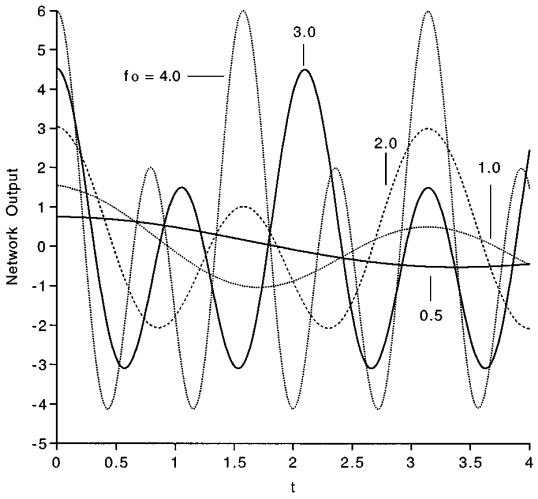

FIG. 6. Heart vibrations. $Z_{\text{out}}(t)$ plots for different f_0 values (404 data points).

In general, any cost function $F(x_i)$ that satisfies Eq. (1), can be approximated accurately by Z_{out} if training succeeds in reducing the associated E_{av} to a sufficiently small value below 10^{-2}. A faster rate of reduction is achieved if the NN has the correct number of hidden neurons and the appropriate α and C_h values are used. Getting the right D and C_h values is done by trial and error and could be laborious especially when the values of $(M+K+1)$ and D are large—experience in NN design is often crucial. In the CNR problem,we used $C_h=\pi$, although putting $C_h=1$, still achieves the same order of reduction for E_{av} but at a larger p value.

Solving DE's by a trained NN has the following distinct advantages: (1) A compact form of the solution is derivable since finite differences are not utilized, (2) speed, and (3) solution search is direct and easy because coordinate transformations are not needed, unlike in traditional methods [15].

[1] G. Arfken, *Mathematical Methods for Physicists*, 3rd ed. (Academic New York, 1985), p. 945.
[2] S. Haykin, *Neural Networks* (Maxwell Macmillan, New York, 1994).
[3] T. Khanna, *Foundations of Neural Networks* (Addison-Wesley, Reading, MA, 1990).
[4] T. Watkin and A. Rau, Rev. Mod. Phys. **65**, 499 (1993).
[5] C. Bishop, Rev. Sci. Instrum. **65**, 1803 (1994).
[6] M. Soriano and C. Saloma, Bioimaging **3**, 168 (1995).
[7] E. Bagarinao and C. Saloma, Phys. Rev. E **54**, 5516 (1996).
[8] F. Girosi and T. Poggio, in *Neural Networks*, edited by P. Antogneti and V. Milutinovic (Prentice-Hall, New York, 1991), Vol. 1.
[9] The derivatives are calculated as: $\partial Z_{\text{out}}/\partial y_r^{\text{in}}=\Sigma_h C_h W_h^{hi}(\partial y_h^{hi}/\partial y_r^{\text{in}})=\Sigma_h C_h W_h^{hi}(W_{hr}^{\text{in}}\Sigma_r[\cos(W_{hr}^{\text{in}}y_\rho^{\text{in}})-\sin(W_{hr}^{\text{in}}y_r^{\text{in}})])$.
[10] Traditional numerical methods (e.g., shooting, finite differences, and Runge-Kutta) cannot solve the DE because $F(R,H)$ is unknown and the initial value condition cannot be determined from the relation that $F(R,H)$ is minimum when $H=1.847R$.
[11] G. Zou and H. Wu, J. Theor. Biol. **172**, 347 (1995).
[12] R. Ripley, J. R. Statist. Soc. **B39**, 172 (1977).
[13] L. Glass, Phys. Today **50** (8), 40 (1996).
[14] W. Press, B. Flannery, S. Teukolsky and W. Vetterling, *Numerical Recipes: The Art of Scientific Computing* (Cambridge University Press, New York, 1986).
[15] B. Ph. van Milligen, V. Tribaldos, and J. Jimenez, Phys. Rev. Lett. **75**, 3594 (1995).