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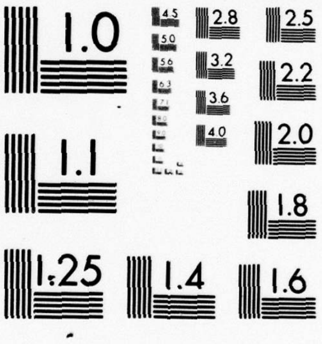

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MODELING FLUCTUATIONS IN MACROSCOPIC SYSTEMS

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April 1979

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ABSTRACT

Macroscopic systems are often modeled by deterministic differential equations (DDE), such as $\dot{x}=f(x,t)$. Here, $x(t)$ is a macrovariable and represents an average over some set of ensembles. A possible extention of such a model to include fluctuations is to assume that a random variable $X(t)$ satisfies a stochastic differential equation (SDE), $\dot{X}=f(X,t)+a(X,t)\xi(t)$. In some sense, $x(t)$ should be the average of $X(t)$. If f is linear and $a(X,t)$ is a constant then $E\{X(t)\}=x(t)$. If $f(X,t)$ is non-linear, then $E\{f(X,t)\} \neq f(E(X),t)$ generally and some authors feel that the SDE is not a correct extension of the DDE. A procedure will be introduced here so that an appropriate conditional average of $X(t)$ is $x(t)$. Thus, there is an underlying consistency between the deterministic and stochastic formulations. The procedure also provides a prescription for the calculation of $a(X,t)$, which is usually not constant if $f(x,t)$ is non-linear. Two examples are studied to illustrate the application of the procedure. First, the logistic equation of population dynamics is studied in deterministic and stochastic versions. Second, stochastic effects on a chemical oscillator are analyzed.

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INTRODUCTION

Very often, macroscopic equations are modeled by differential equations of the form:

$$\frac{dx}{dt} = f(x,t) \qquad x(0) = x_0 \ . \tag{1}$$

In equation 1, $x = (x_1, x_2, \ldots, x_n)$ is a vector in R^n. Since the system of interest in macroscopic, $x(t)$ is regarded as an "ensemble average" of some sort. Namely, $x(t)$ is the average of some random variable $X(t)$. A possible way to find the equation that $X(t)$ satisfies is to add a random term to equation 1, so that $X(t)$ satisfies the Langevin equation:

$$\frac{dX}{dt} = f(X,t) + a(X,t)\xi(t) \ , \qquad X(0) = x_0 \ . \tag{2}$$

In equation 2, $\xi(t)$ is assumed to be a zero mean random process with correlation function $\phi(t,\tau) = E\{\xi(t+\tau)\xi(t)\}$. The connection between the two equations is not automatically clear and, in fact, is the subject of controversy [1,2]. In this paper, an attempt is made to relate the two equations. In particular, since experience shows that phenomenological equations are often deterministic (i.e., of the form (1)), "the mean" of $X(t)$ in equation 2 should be $x(t)$ in equation 1. The exact sense of "the mean" will be clarified in this paper.

THE LINEAR CASE

The situation is simple (and classical, see references 3 and 4) when $f(x,t) = \Lambda x$, where Λ is a constant matrix. Assuming that $a(X,t) = A$, a constant, the stochastic equation 2 becomes:

$$\frac{dX}{dt} = \Lambda X + A\xi(t) \tag{3}$$

Averaging both sides in equation 3 gives:

$$\frac{d\langle X\rangle}{dt} = \Lambda\langle X\rangle \qquad \langle X(0)\rangle = x_0 , \tag{4}$$

where $\langle X\rangle = E\{X(t)|X(0)=x_0\}$. Clearly, in this case $\langle X(t)\rangle = x(t)$.

THE NON-LINEAR CASE

Now consider equation 2 when $f(\cdot,t)$ is non-linear. Averaging this equation gives:

$$\frac{d\langle X\rangle}{dt} = \langle f(X,t)\rangle + \langle a(X,t)\xi(t)\rangle . \tag{5}$$

When $f(\cdot,t)$ is non-linear

$$\langle f(X,t)\rangle \neq f(\langle X\rangle,t) , \tag{6}$$

except in special cases. Also note that in general,

$$\langle a(X,t)\xi(t)\rangle \neq 0 . \tag{7}$$

Thus, one concludes that in this case, $\langle X(t)\rangle \neq x(t)$ and that there is no simple relationship between equations 2 and 1.

Should equation 2 be rejected as meaningless? One could retrieve equation 1 from equation 2, by assuming that $a(X,t) \propto 1/V$ where V is a measure of the size of the system. Then, as $V\to\infty$, equation 2 collapses into equation 1. Such a procedure is used in statistical mechanics, of course, and is called the "thermodynamic limit" (with additional assumptions). In this paper, a different resolution of the paradox is given.

INITIALLY AND CONTINUOUSLY CONDITIONED MEANS*

The mean introduced in the previous section will be called the initially conditioned mean since it is defined as:

$$\langle X(t)\rangle = E\{X(t)|X(0)=x_0\} \quad . \tag{8}$$

A second type of mean will be introduced now (also see reference 6). To motivate the results given below, note that equation 1 is equivalent to the difference equation:

$$x(t+\Delta t) - x(t) = f(x,t)\Delta t + o(\Delta t) \quad , \tag{9}$$

where $o(Z)/Z\to 0$ as $Z\to 0$. The interpretation of equation 9 is that given $x(t) = x$, the increment in $x(t)$, $x(t+\Delta t) - x(t)$, is $f(x,t)\Delta t + o(\Delta t)$.

Denote by $\bar{X}(t)$ the continuously conditioned mean. Namely, define $\bar{X}(t)$ incrementally by:

$$\bar{X}(t+\Delta t) - \bar{X}(t) \equiv E\{X(t+\Delta t)-X(t)|X(t)=x\} \quad . \tag{10}$$

Now consider equation 2, given that $X(t) = x$. This equation can be rewritten as:

$$X(t+\Delta t) - X(t) = f(x,t)\Delta t + a(x,t)\xi(t)\Delta t + o(\Delta t) \quad . \tag{11}$$

---

[*] These terms are due D.T. Gillespie, also see reference 5.

Next, take the mean of equation 11, conditioned on $X(t) = x$. Then, one finds:

$$\bar{X}(t+\Delta t) - \bar{X}(t) = f(x,t)\Delta t + o(\Delta t). \tag{12}$$

The right-hand sides of equations 2 and 9 are identical, so that one concludes that:

$$\bar{X}(t) = x(t). \tag{13}$$

Thus, the deterministic variable $x(t)$ is the continuously conditioned mean of $X(t)$. In order to exploit this concept, one needs a fluctuation algorithm for the calculation of the continuously conditioned mean. In the next section, such algorithms will be discussed. These algorithms also lead to a prescription for the calculation of $a(X,t)$. From equation 11, one has that, given $X(t) = x$:

$$[X_i(t+\Delta t)-X_i(t)][X_j(t+\Delta t)-X_j(t)] = [f_i(x,t)\Delta t+a_{ik}(x,t)\xi_k(t)\Delta t+o(\Delta t)]$$
$$[f_j(x,t)\Delta t+a_{jk}(x,t)\xi_k(t)\Delta t+o(\Delta t)]. \tag{14}$$

The notation used in equation 14 is that of summation over repeated indices, so that:

$$a_{ik}(x,t)\xi_k(t) = \sum_{k=1}^{n} a_{ik}(x,t)\xi_k(t) \quad . \tag{15}$$

If the noise process is to be noticable on deterministic time scales, one assumes that:

$$E[\xi_k(t)\xi_\ell(t)(\Delta t)^2] = \sigma_{k\ell}^2 \Delta t \quad . \tag{16}$$

Equation 16 is satisfied by Gaussian white noise and related approximating process (e.g., reference 7). Set:

$$\Delta X_i = X_i(t+\Delta t) - X_i(t) \quad . \tag{17}$$

Taking the continuously conditioned mean of equation 14 and using equations 15 and 16 gives:

$$\begin{aligned} \lim_{\Delta t \downarrow 0} \left[\frac{1}{\Delta t} E\{\Delta X_i \Delta X_j | X(t)=x\} \right] &= \lim_{\Delta t \downarrow 0} a_{ik}(x,t) a_{j\ell}(x,t) \\ &\quad E\{\xi_k(t)\Delta t \xi_\ell(t)\Delta t\} \\ &= a_{ik}(x,t) a_{j\ell}(x,t) \sigma_{k\ell}^2 \end{aligned} \tag{18}$$

Since σ_k^2 is presumed to be known, if the left-hand side of equation 18 is known, then the matrix $a_{ij}(x,t)$ can be determined.

Also note that in this formulation $a_{ij}(x,t)$ cannot be chosen arbitrarily but is defined by equation 18. Thus, by requiring the deterministic variable to be the continuously conditioned mean, the coefficient of the noise term is also fixed. Hence, it is not proper to assume in equation 2 that $a(x,t) = A$, a constant.

PHENOMENOLOGICAL EQUATIONS
AND FLUCTUATION ALGORITHMS

In this section, two formalisms are given for the calculation of moments of ΔX_i . In the first algorithm, one assumes no knowledge of the mechanism underlying the macroscopic equations. In the second algorithm, one assumes that the underlying mechanism is known. Application of each algorithm is illustrated in the next section.

FLUCTUATION ALGORITHM FOR PROCESSES WITHOUT UNDERLYING MECHANISM

Often, the macroscopic equation is derived without knowledge of the underlying mechanism. The fluctuation algorithm is derived as follows. Assume that:

$$f_i(x,t) = f_i^+(x,t) - f_i^-(x,t) \quad , \tag{19}$$

with $f_i^+(x,t) \geq 0$, $f_i^-(x,t) \geq 0$. Then, assume that:

$$\Pr\{\Delta X_i=1|X(t)=x\} = f_i^+(x,t)\Delta t + o(\Delta t) \tag{20}$$

$$\Pr\{\Delta X_i=1|X(t)=x\} = f_i^-(x,t)\Delta t + o(\Delta t) \tag{21}$$

$$\Pr\{\text{all other transitions}\} = o(\Delta t) \ . \tag{22}$$

Then, one finds:

$$E\{X_i(t+\Delta t)-X_i(t)|X(t)=x\} = [f_i^+(x,t)-f_i^-(x,t)]\Delta t + o(\Delta t) \ , \tag{23}$$

and the matrix $[a_{ij}(x,t)]$ is diagonal with elements:

$$a_{ii}(x,t) = \left[\frac{f_i^+(x,t) + f_i^-(x,t)}{\sigma_{ii}^2}\right]^{\frac{1}{2}} . \qquad (24)$$

Equation 24 is derived as follows. From equations 20-23,

$$E\{\Delta X_i \Delta X_j | X(t)=x\} = o(\Delta t) \quad , \qquad (25)$$

if $i \neq j$. When $i = j$,

$$E\{\Delta X_i^2 | X(t)=x\} = [f_i^+(x,t) + f_i^-(x,t)]\Delta t + o(\Delta t). \qquad (26)$$

Using equation 18 gives:

$$f_i^+(x,t) + f_i^-(x,t) = a_{ii}(x,t)^2 \sigma_{ii}^2 \quad , \qquad (27)$$

from which equation 24 follows.

FLUCTUATION ALGORITHM FOR PROCESSES UNDERLYING MECHANISM

In many chemical and physical processes, one can use "elementary events" to describe the macroscopic events (see below for an example). Assume that there are M "elementary events" that can be modeled as:

$$\Pr\{\Delta X_1 = r_1^k, \Delta X_2 = r_2^k, \ldots, \Delta X_n = r_n^k | X(t)=x\} = \lambda_k(x,t)\Delta t + o(\Delta t) \qquad (28)$$

$$k = 1,2,\ldots,M .$$

From equation 28, one immediately obtains:

$$E\{\Delta X_i | X(t)=x\} = r_i^k \lambda_k(x,t)\Delta t + (\Delta t) \quad . \tag{29}$$

For consistency of deterministic and stochastic equations, one requires that:

$$f_i(x,t) = r_i^k \lambda_k(x,t) \quad . \tag{30}$$

From equation 28, one also immediately obtains:

$$E\{\Delta X_i \Delta X_j | X(t)=x\} = r_i^k r_j^k \lambda_k(x,t)\Delta t + o(\Delta t) \quad . \tag{31}$$

Hence, the matrix $a_{ij}(x,t)$ is determined as the solution of:

$$r_i^k r_j^k \lambda_k(x,t) = a_{im}(x,t) a_{j\ell}(x,t) \sigma^2_{\ell m} \quad . \tag{32}$$

The fluctuation algorithm give here is equivalent to Keizer's "fluctuation dissipation postulates" (reference 1).

"SURE" TERMS IN THE MACROSCOPIC EQUATIONS

Sometimes a deterministic term will appear in the macroscopic equations. A typical case would be that $f(x,t)$ has a component of the form:

$$f_i(x,t) = f_{i0}(t) + f_{i1}(x,t) \quad , \tag{33}$$

where $f_{i0}(t)$ is deterministic. In this case, one rewrites equation 2 as:

$$\frac{dX_i}{dt} - f_{i0}(t) = f_{i1}(X,t) + a_{ik}(X,t)\xi_k(t) \quad . \tag{34}$$

From equation 34, it is apparent that the fluctuation algorithms described above should be applied to the quantity:

$$X_i(t+\Delta t) - X_i(t) - f_{i0}(t)\Delta t \quad , \tag{35}$$

(also, see reference 5).

EXAMPLES OF THE FLUCTUATION ALGORITHMS

In this section, two examples of the fluctuation algorithms are discussed. Two other examples are the mean field ferromagnet and the laser (references 8 and 9).

LOGISTIC EQUATION OF POPULATION DYNAMICS

The following equation is often used as a model in theoretical ecology (e.g., reference 10):

$$\frac{dx}{dt} = rx\left(1 - \frac{x}{K}\right) \quad . \tag{36}$$

In this equation, $x(t)$ represents the size of the population at time t. R. May has suggested that the variable $X(t)$ satisfies the following stochastic equation (reference 10):

$$\frac{dX}{dt} = rX\left(1 - \frac{X}{K}\right) + \alpha X\xi(t) \quad , \tag{37}$$

where $\xi(t)$ is Gaussian white noise and α is a constant.

If the first fluctuation algorithm is applied, then it is assumed that:

$$\text{Prob}\{X(t+\Delta t)-X(t)=1 \,|\, X(t)=x\} = rx\Delta t + o(\Delta t) \tag{38}$$

$$\text{Prob}\{X(t+\Delta t)-X(t)-1 \,|\, X(t)=x\} = \frac{rx^2}{K}\Delta t + o(\Delta t) \tag{39}$$

$$\text{Prob}\{\text{all other transitions}\} = o(\Delta t) \quad . \tag{40}$$

Equations 38-40 correspond to a linear birth-quadratic death process. Hence:

$$E\{(\Delta X)^2 | X(t)=x\} = rx\left(1 + \frac{x}{K}\right)\Delta t + o(\Delta t) \; . \tag{41}$$

For Gaussian white noise $\sigma^2 = 1$, so that equation 18 becomes:

$$rx\left(1 + \frac{x}{K}\right) = [a(x,t)]^2 \; . \tag{42}$$

Hence, the consistent extension of the logistic equation 36 is not equation 37 but is:

$$\frac{dX}{dt} = rX\left(1 - \frac{X}{K}\right) + \left[rX\left(1 + \frac{X}{K}\right)\right]^{\frac{1}{2}} \xi(t) \; . \tag{43}$$

The Fokker-Planck equation for the probability density of the process described by equation 37 is (see reference 7):

$$\frac{\partial}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}(aX^2\rho) - \frac{\partial}{\partial x}\left[rX\rho\left(1 - \frac{X}{K}\right)\right] \tag{44a}$$

While the Fokker-Planck equation for the density fo the process described by equation 43 is:

$$\frac{\partial \rho}{\partial t} = \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[rX\rho\left(1 + \frac{X}{K}\right)\right] - \frac{\partial}{\partial X}\left[rX\rho\left(1 - \frac{X}{K}\right)\right] \; . \tag{44b}$$

Both of the above equations are singular diffusion equations (reference 11). There is, however, a major difference in that the diffusion coefficient of equation 44a goes as X^2 for small X , but that of equation 44b goes as X for small X . Many of th results described in reference 10 are due to the high singularity of the diffusion coefficient. Some of these results would not be obtained if equation 43 were used instead of equation 37.

CHEMICAL OSCILLATOR WITH FLUCTUATIONS

The following reaction mechanism has been studied by I. Prigogine and his collaborators (reference 12) as a prototype chemical oscillator.

$$\begin{aligned} & A \to X_1 \\ & X_1 + B \to X_2 \\ & 2X_1 + X_2 \to 3X_1 \\ & X_1 \to P \end{aligned} \tag{45}$$

Assume that the concentrations of A and B , denoted by α, β respectively, are constant. Let x_i denote the concentration of species i . The phenomenological rate equations are:

$$\begin{aligned} \frac{dx_1}{dt} &= \alpha + x_1^2 x_2 - (\beta+1) x_1 \\ \frac{dx_2}{dt} &= \beta x_1 - x_1^2 x_2 \end{aligned} \tag{46}$$

These equations can have oscillatory solutions (figures 1 and 2). Hence, one concludes that if the stochastic problem is properly formulated, then the continuously conditioned means $\overline{X_1(t)}$, $\overline{X_2(t)}$ are also oscillatory.

Now consider the formulation of the stochastic equations. The equations for $X_1(t)$ and $X_2(t)$ take the form (assuming that α is a sure term):

$$\frac{dX_1}{dt} - \alpha = X_1^2X_2 - (\beta+1)X_1 + [a_{11}(X_1,X_2,t)\xi_1(t) + a_{12}(X_1,X_2,t)\xi_2(t)] \tag{47}$$

$$\frac{dX_2}{dt} = \beta X_1 - X_1^2X_2 + [a_{12}(X_1,X_2,t)\xi_2(t) + a_{22}(X_1,X_2,t)\xi_3(t)]. \tag{48}$$

Here, $\xi_1(t)$, $\xi_2(t)$, $\xi_3(t)$ are independent stochastic processes. They need not be Gaussian white noise.

The second fluctuation algorithm of the previous section applies in this case. From the reaction mechanism (equation 45) the following transition probabilities are constructed:

$$\Pr\{(\Delta X_1-\alpha\Delta t)=1,\ \Delta X_2=-1 \mid X_1(t)=x_1,\ X_2(t)=x_2\} = x_1^2x_2\Delta t+o(\Delta t) \tag{49}$$

$$\Pr\{(\Delta X_1-\alpha\Delta t)=-1,\ \Delta X_2=0 \mid X_1(t)=x_1,\ X_2(t)=x_2\} = x_1\Delta t+o(\Delta t) \tag{50}$$

$$\Pr\{(\Delta X_1-\alpha\Delta t)=-1,\ \Delta X_2=1 \mid X_1(t)=x_1,\ X_2(t)=x_2\} = \beta x_1\Delta t+o(\Delta t) \tag{51}$$

$$\Pr\{\text{all other transitions}\} = o(\Delta t) \tag{52}$$

From equations 49-52, one finds that:

$$E\{(\Delta X_1-\alpha\Delta t)|X_1(t)=x_1,\ X_2(t)=x_2\} = x_1^2x_2\Delta t-(\beta+1)x_1\Delta t + o(\Delta t) \quad (53)$$

$$E\{\Delta X_2|X_1(t)=x_1,\ X_2(t)=x_2\} = \beta x_1\Delta t - x_1^2x_2\Delta t + o(\Delta t)\ , \quad (54)$$

So that the deterministic equations are obtained as the conditional mean.

Now consider calculation of the matrix (a_{ij}). From equations 49-52:

$$E\{(\Delta X_1-\alpha\Delta t)^2|X_1(t)=x_1,\ X_2(t)=x_2\} = [x_1^2x_2 +(\beta+1)x_1]\Delta t + o(\Delta t) \quad (55)$$

Since $E\{\Delta X_1|X(t)=x\} = 0(\Delta t)$, equation 55 is rewritten as:

$$E\{(\Delta X_1)^2|X_1(t)=x_1,\ X_2(t)=x_2\}+o(\Delta t) = [x_1^2x_2+(\beta+1)x_1]\Delta t+o(\Delta t) \quad (56)$$

Clearly,

$$E\{(\Delta X_2)^2|X_1(t)=x_1,\ X_2(t)=x_2\} = [x_1^2x_2+\beta x_1]\Delta t + o(\Delta t)\ . \quad (57)$$

Finally,

$$E\{(\Delta X_1-\alpha\Delta t)\Delta X_2|X_1(t)=x_1,\ X_2(t)=x_2\} = -(x_1^2x_2+\beta x_1)\Delta t+o(\Delta t). \quad (58)$$

Expanding the product in the left-hand side of equation 58 gives

$$E\{\Delta X_1\Delta X_2|X_1(t)=x_1,\ X_2(t)=x_2\}+o(\Delta t) = -(x_1^2x_2+\beta x_1)\Delta t+o(\Delta t). \quad (59)$$

The matrix (a_{ij}) is now determined from equation 18.

Since the continuously conditioned mean oscillates, it is interesting to wonder if the initially conditioned mean also oscillates (also see references 5 and 13). In figures 3 and 4, the initially conditioned means $\langle X_1(t)\rangle$ and $\langle X_2(t)\rangle$ are plotted. These means were evaluated by numerical solution of equations 47 and 48. It is seen that these menas decay and seem to approach a constant. The technique of reference 13 can be used to check the numerical results as follows. If the initially conditioned mean of equations 47 and 48 is taken, one obtains:

$$\frac{d}{dt}\langle X_1\rangle = \langle X_1^2X_2\rangle + \alpha - (\beta+1)\langle X_1\rangle + \langle a_{11}(X_1,X_2,t)\xi_1(t) + a_{12}(X_1,X_2,t)\xi_2(t)\rangle \tag{59}$$

$$\frac{d}{dt}\langle X_2\rangle = \beta\langle X_1\rangle - \langle X_1^2X_2\rangle + \langle a_{12}(X_1,X_2,t)\xi_2(t) + a_{22}(X_1,X_2,t)\xi_3(t)\rangle \; . \tag{60}$$

Now assume that as $t\to\infty$

$$\frac{d}{dt}\langle X_i\rangle \to 0 \qquad i = 1,2 \tag{61}$$

and

$$\langle a_{ik}(X_1,X_2,t)\xi_k(t)\rangle\to 0 \qquad i,k = 1,2 \; . \tag{62}$$

Equations 61 and 62 are assumptions and are not derived from any of the above results. Denote by $\langle X_i \rangle_\infty$ as the limiting value of $\langle X_i(t) \rangle$ as $t \to \infty$. Then, from equations 59 and 60:

$$0 = \langle X_1^2 X_2 \rangle_\infty + \alpha - (\beta+1)\langle X_1 \rangle_\infty \tag{63}$$

$$0 = \beta\langle X_1 \rangle_\infty - \langle X_1^2 X_2 \rangle_\infty \quad . \tag{64}$$

Hence, one finds,

$$\langle X_1 \rangle_\infty = \alpha \quad , \tag{65}$$

which appears to be in agreement with the numerical result in figure 3. Equations 63 and 64 cannot be used to provide information about $\langle X_2 \rangle_\infty$.

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CAPTIONS:

Fig. 1: The continuously conditioned mean $\overline{X_1(t)}$ for the chemical oscillator (45), with $\alpha=1$, $\beta=3$.

Fig. 2: The continuously conditioned mean $\overline{X_2(t)}$.

Fig. 3: The initially conditioned mean $\langle X_1(t)\rangle$ for the chemical oscillator (45). An ensemble of 500 phase points was used.

Fig. 4: The initially conditioned mean $\langle X_2(t)\rangle$.

Fig 1

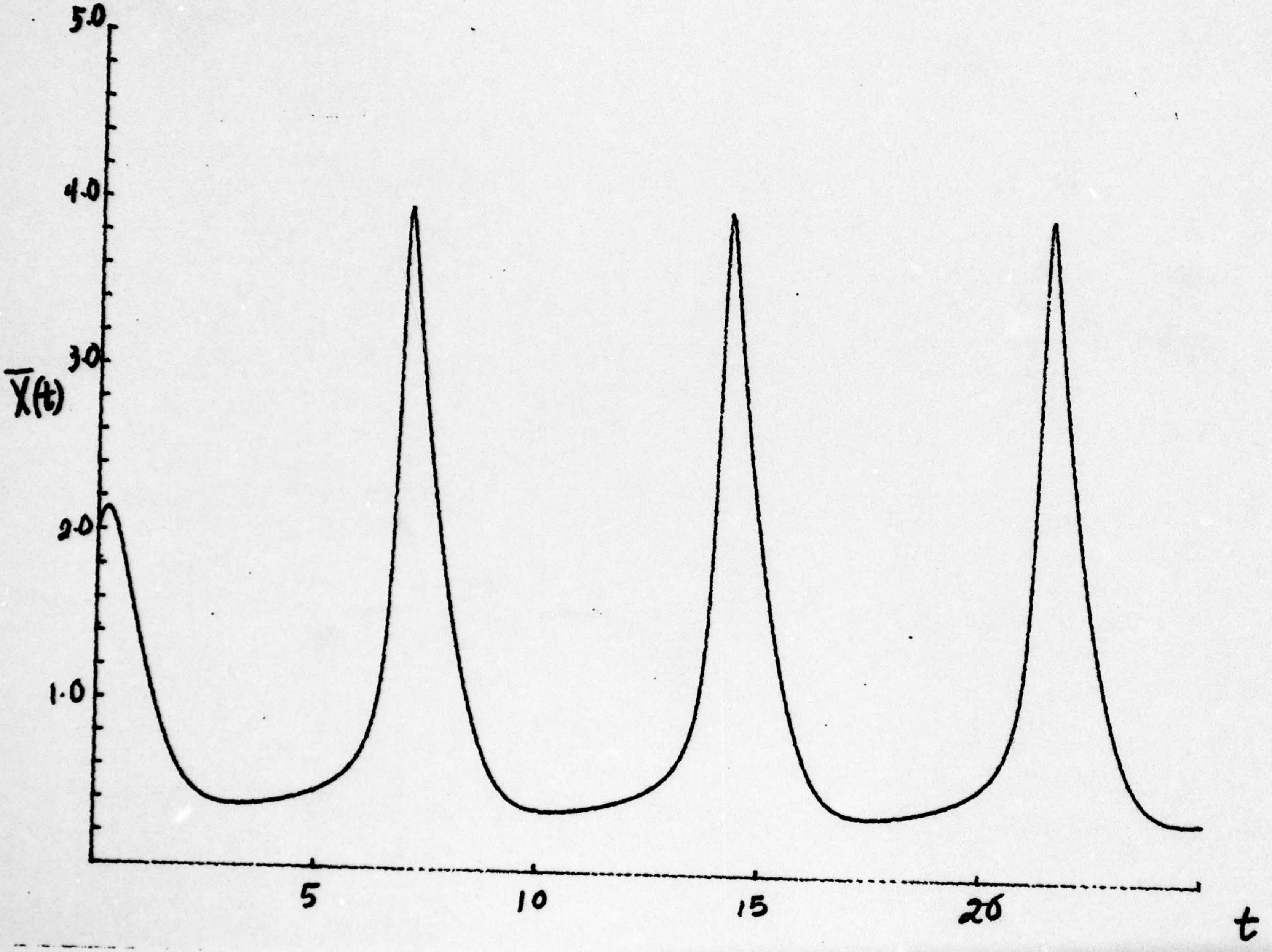


Fig 2

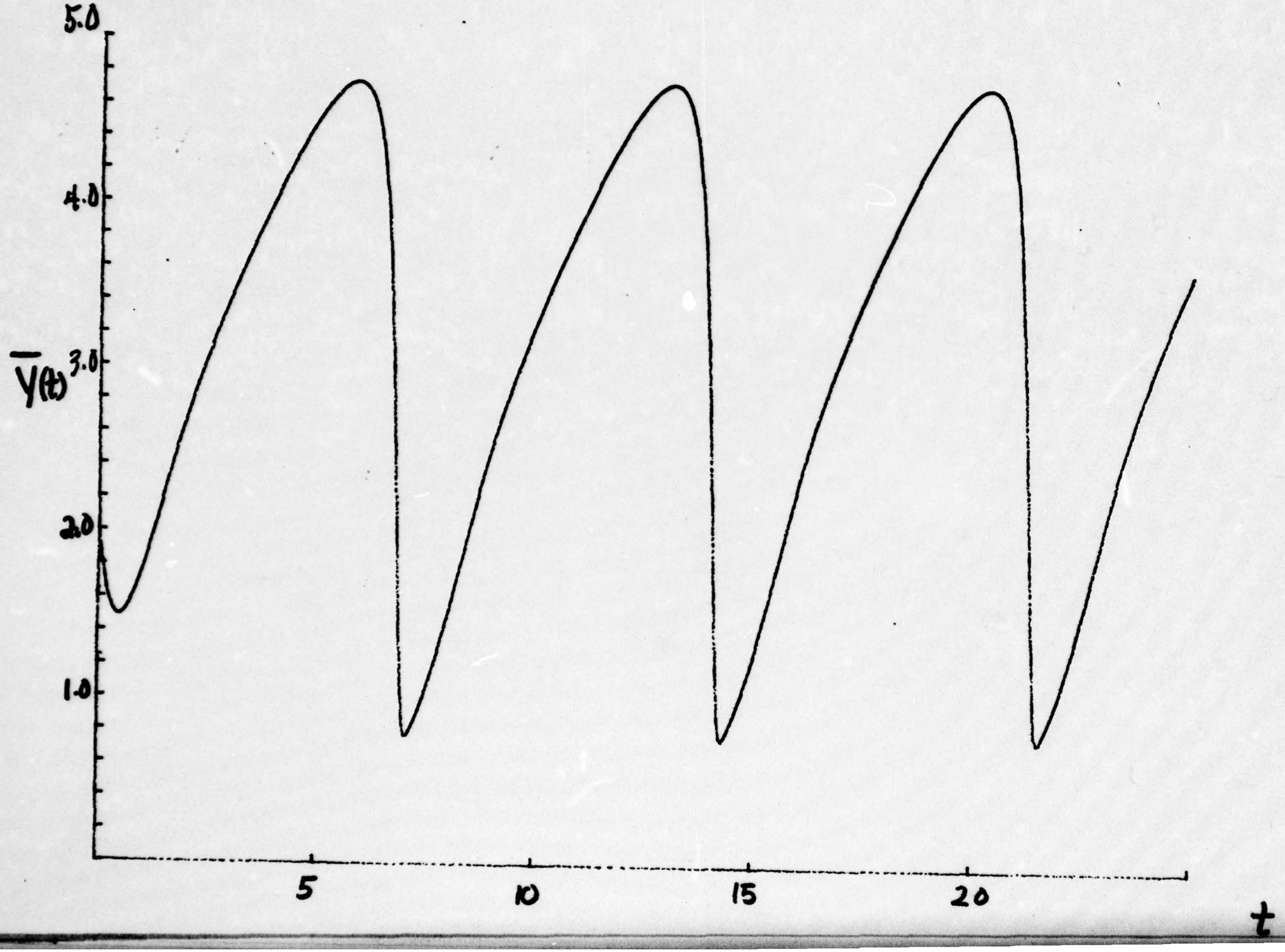


Fig. 3

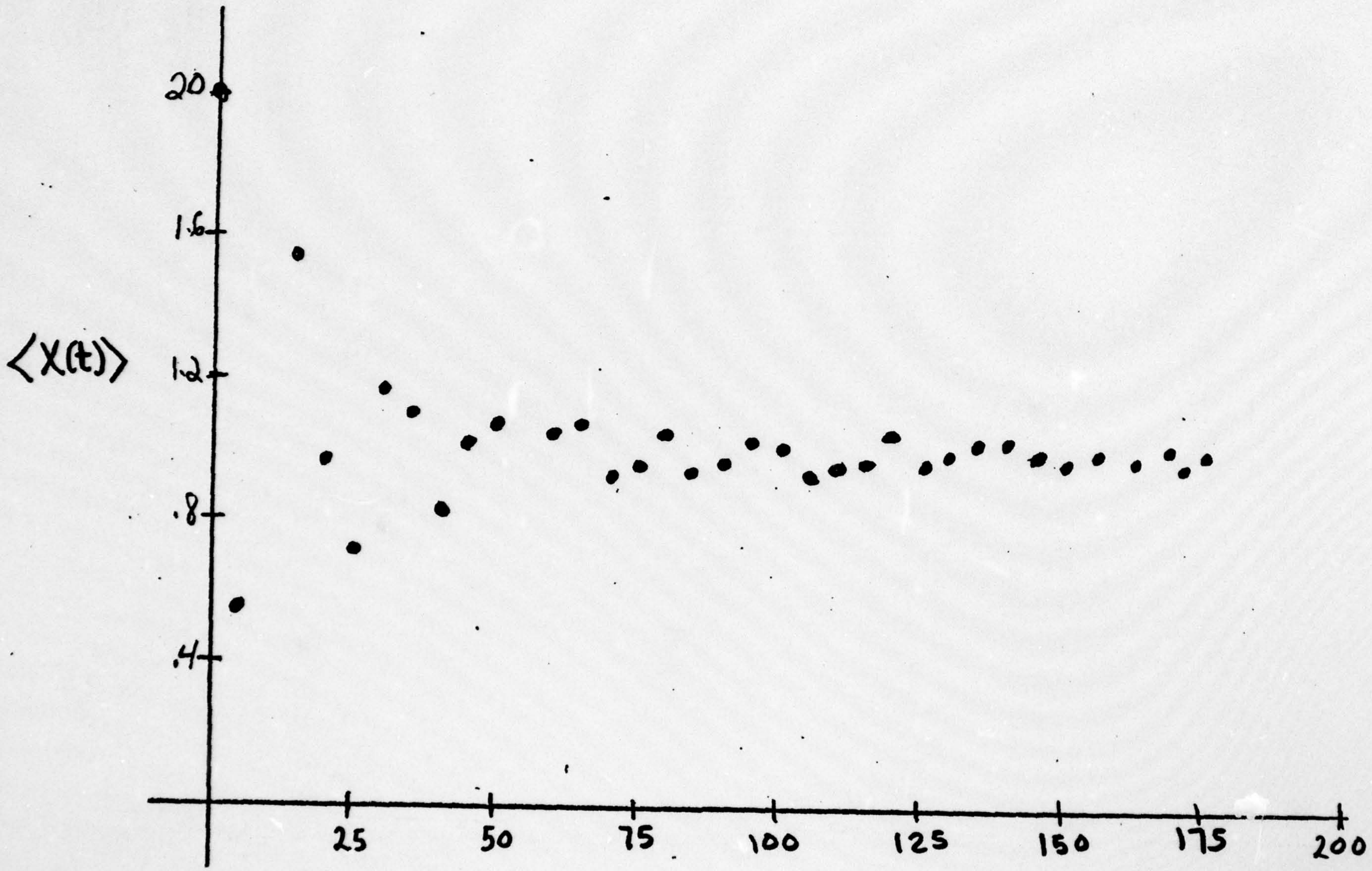
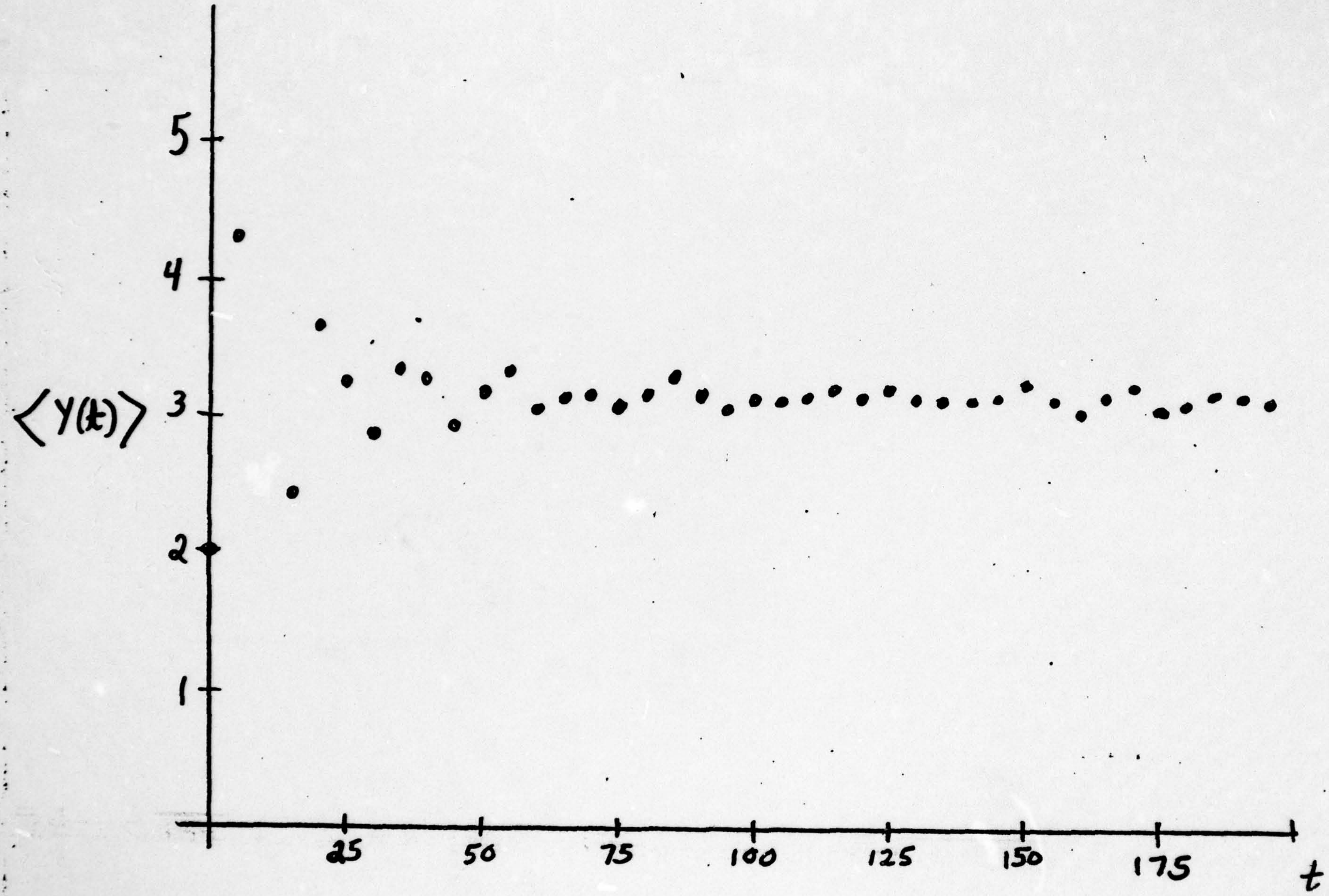


Fig. 4



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