Working Paper

On a problem of source reconstruction for parabolic equation

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WP-96-38
April 1996

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Preface

In the present paper the problem of reconstruction of the right-hand side of an advection-diffusion equation is considered. This type of equation is used in many models of contamination transport in domains such as air, groundwater and surface water. Using the method of conjugate equations, one can reduce the problem to an integral equation of the first kind. In the paper a discrete analog of this integral equation is constructed on the basis of discretization of the initial advection-diffusion equation and the usage of the conjugate equation technique. For solving the obtained discrete analog of the integral equation Tikhonov's method of regularization is applied. The parameter of regularization is chosen in accordance with the residual principle. Series of numerical calculations show efficiency of the method.

The paper continues research on inverse problems for distributed systems started at IIASA's project on Dynamic Systems in 1994.

Contents

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Introduction

Groundwater plays an important role as a major source of high-quality drinking water. However, contamination both from agricultural activities and waste disposals often endanger groundwater. The management and remediation of groundwater contamination problems are among the more complex tasks in environmental management and technology. To evaluate pollution problems many mathematical models differing in complexity and details have been developed. More detailed models describe groundwater flow and contamination transport. In this paper we consider a mathematical model describing contamination transport in an unconfined aquifer under assumption that water table level and velocities of the flow are known. One of the problems of interest for groundwater management and remediation is source reconstruction. In this paper the possibility of satisfactory reconstruction of the source intensity through observations is shown. This problem is an ill-posed problem; for its solving a special mathematical method, based on the method of conjugate equations and Tikhonov's regularization technique, is suggested.

1 Description of the Mathematical Model

A mathematical model describing a contamination process in a two-dimensional (2D) unconfined aquifer is represented by a nonstationary partial differential equation of parabolic type

$$\begin{aligned} \frac{\partial(\Theta \cdot (H - h_b) \cdot C)}{\partial t} &+ \operatorname{div}(\epsilon \cdot (H - h_b) \cdot V \cdot C) + \Theta \cdot (H - h_b) \cdot \sigma \cdot C \\ &= \operatorname{div}(\epsilon \cdot (H - h_b) \cdot D \cdot \operatorname{grad} C) + Q_C, \end{aligned} \tag{1.1}$$

where

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t	=	time,
x, y	=	Cartesian coordinates,
$V = (v_x, v_y)$	=	components of depth-averaged horizontal fluid velocities in x, y directions,
$H = H(x, y, t)$	=	aquifer height,
$C = C(x, y, t)$	=	concentration of specific constituent under consideration,
$D = D(x, y, t)$	=	tensor of hydrodynamic dispersion,
$\epsilon = \epsilon(x, y, t)$	=	kinematic porosity,
$\theta = const_1$	=	adsorption coefficient,
$\sigma = const_2$	=	concentration decay rate,
$\Theta = \Theta(x, y, t)$	=	$\epsilon + (1 - \epsilon) \cdot \theta$, specific retardation factor.

The right-hand side $Q_C = Q_C(x, y, t)$ represents a source of contamination.

The 2D convection-dispersion mass transport equation (1.1) allows one to analyze a situation after an event on the basis of measured data. It is given in a general form and reflects the effects of convection, dispersion, adsorption, decay, as well as sources and sinks. A specification of boundary and initial conditions is determined by the nature of a problem under investigation.

In the present paper for equation (1.1) a problem of contaminant source reconstruction is considered. Methodologically the problem belongs to the category of inverse problems for dynamical systems. The problem consists in finding a time-varying intensity of a source on the basis of concentration measurements in a certain domain. In general, a solution of the problem is not a unique one (see, e.g., Osipov, 1989). However in some particular cases, for example if

$$Q_C(x, y, t) = z(t)\, \omega(x, y), \qquad (1.2)$$

where $\omega(x, y)$ is a given function, the uniqueness of the time component $z(t)$ can be obtained.

In this paper we demonstrate a satisfactory reconstruction of source's time component $z(t)$ in a model situation. The paper follows Kryazhimskii, Maksimov, and Samarskaia (1995).

2 Problem Formulation

Let equation (1.1) be specified as a 2D linear partial differential equation of parabolic type with constant coefficients in a rectangular domain G

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} + v_y \frac{\partial C}{\partial y} + \gamma\, C = D \frac{\partial^2 C}{\partial x^2} + D \frac{\partial^2 g}{\partial y^2} + z(t)\, \omega(x, y) \quad \text{in G;} \qquad (2.1)$$

here

$$v_x = const_3,\; v_y = const_4,\; \gamma = const_5,\; D = const_6,$$
$$G = \{\, (x, y) :\; 0 \le x \le a,\;\; 0 \le y \le b \,\},$$

functions $\omega(x, y)$ and $z(t)$ are piece-wise smooth. On the boundary Γ of the domain G we fix the boundary condition

$$C(t, x, y)\, |_\Gamma = 0. \qquad (2.2)$$

The initial condition for equation (2.1) is

$$C(0, x, y) = 0. \tag{2.3}$$

Let a non-negative piece-wise continuous function $p(x, y)$ on G define the domain of contaminant concentration observations

$$P = \{\ (x, y) :\ (x, y) \in G,\ \ p(x, y) \geq\ 0\ \}. \tag{2.4}$$

Assume that observation results are known and given by function

$$u(t) = \int\int_G C(t, x, y)\, p(x, y)\, dxdy. \tag{2.5}$$

In practice function $u(t)$ is defined with a known accuracy. The problem is to reconstruct $z(t)$ on the basis of $u(t)$ and all other parameters of equation (2.1). This problem is ill-posed, therefore one needs using special stable methods to find an approximate solution. Let us give a relationship between the time component $z(t)$ of the source Q_C and the results of observations $u(t)$. For this purpose following Kryazhimskii and Osipov, 1993, Kryazhimskii, Maksimov, and Samarskaia, 1995 we apply the method of conjugate problem (Lions, 1971, Marchuk, 1992).

Consider the conjugate equation

$$\frac{\partial g}{\partial t} - v_x\, \frac{\partial g}{\partial x} - v_y\, \frac{\partial g}{\partial y} + \gamma\, g = D\, \frac{\partial^2 g}{\partial x^2} + D\, \frac{\partial^2 g}{\partial y^2} \tag{2.6}$$

in G with the following boundary and initial conditions:

$$\begin{aligned} g(t, x, y)\mid_\Gamma &= 0, \\ g(0, x, y) &= p(x, y). \end{aligned} \tag{2.7}$$

Let $C(\tau, x, y)$ and $g(\tau, x, y)$ be respectively the values of the solutions C and g of problems (2.1) - (2.3) and (2.6) - (2.8) at time τ in point (x, y). The integration of $C(\tau, x, y)\ g(\tau, x, y)$ over $[0, t] \times G$ leads to the linear Volterra equation

$$\int_0^t K(t - \tau)\ z(\tau)\ d\tau = u(\tau) \tag{2.8}$$

where kernel K and the right-hand side u have the following form

$$K(t) = \int\int_G g(t, x, y)\, \omega\ dxdy, \tag{2.9}$$

$$\begin{aligned} u(t) &= \int\int_G C(t, x, y)\, p(x, y)\ dxdy - \int\int_G z(t, x, y)\ C(0, x, y)\ dxdy \\ &= \int\int_G C(t, x, y)\, p(x, y)\ dxdy \end{aligned} \tag{2.10}$$

(see the initial condition (2.3)).

The integral equation (2.8) determines an ill-posed problem and therefore requires regularization. Among the practically used algorithms of regularization there are general and special ones. General algorithms are usually based on finding an extremal point of α-parametrical Tikhonov's functional under an appropriate correspondance between the parameter of regularization and the level of data errors. Special algorithms of regularization take into account the main features of concrete problems and therefore can be more efficient in comparison with general ones.

Without specifying conditions for the existence, uniqueness and smoothness of solutions of the equations (1.1) and (2.6) (these issues are studied in Tikhonov and Samarskii, 1963, Lions, 1971, Marchuk, 1992) we shall consider a finite-difference approximation of the initial problem and build a discrete analogue of the integral equation (2.8).

3 Implicit Finite-Difference Scheme

To solve equations (2.1) and (2.6) numerically introduce a time grid ω_τ and a space grid ω_h in the domain G:

$$
\begin{aligned}
\omega_t &= \{t_n = n\,\Delta t,\ \ n = 0,1,2,...,N_t, \Delta t = t_0/N_\tau\},\\
\omega_h &= \{(x_i,y_j) \in G,\ \ x_i = i\Delta x,\ \ y_j = j\Delta y,\\
&\quad \Delta x = l_x/N_x,\ \ \Delta y = l_y/N_y,\ \ i = 0,1,2,...,N_x,\ \ j = 0,1,2,...,N_y\}.
\end{aligned}
$$

Assume the general abbreviated notation

$$
\phi(t_n, x_i, y_j) = \phi^n_{i,j}. \tag{3.1}
$$

Let $v_x \geq 0, v_y \geq 0$. For equation (2.1) we use the implicit finite-difference scheme

$$
\begin{aligned}
\frac{C^{n+1}_{i,j} - C^n_{i,j}}{\Delta t} &+ v_x \frac{C^{n+1}_{i,j} - C^{n+1}_{i-1,j}}{\Delta x} + v_y \frac{C^{n+1}_{i,j} - C^{n+1}_{i,j-1}}{\Delta y} + \gamma\, C^{n+1}_{i,j}\\
&- D\frac{C^{n+1}_{i+1,j} - 2C^{n+1}_{i,j} + C^{n+1}_{i-1,j}}{\Delta x^2}\\
&- D\frac{C^{n+1}_{i,j+1} - 2C^{n+1}_{i,j} + C^{n+1}_{i,j-1}}{\Delta y^2} - z_n\,\omega_{i,j} = 0,
\end{aligned} \tag{3.2}
$$

where $z_n = z(t_n)$, $\omega_{i,j} = \omega(x_i, y_j)$, and assume the homogeneous boundary conditions of the first kind

$$
C_{0,j} = C_{1,j} = C_{N_x,j} = C_{1,N_y} = 0 \tag{3.3}
$$

and the homogeneous initial condition

$$
C^0_{i,j} = 0\ . \tag{3.4}
$$

To solve the conjugate equation (2.6) we use the implicit finite-difference scheme

$$
\begin{aligned}
\frac{g^{n+1}_{i,j} - g^n_{i,j}}{\Delta t} &- v_x \frac{g^{n+1}_{i+1,j} - g^{n+1}_{i,j}}{\Delta x} - v_y \frac{g^{n+1}_{i,j+1} - g^{n+1}_{i,j}}{\Delta y} + \gamma g^{n+1}_{i,j}\\
&- D\frac{g^{n+1}_{i+1,j} - 2g^{n+1}_{i,j} + g^{n+1}_{i-1,j}}{\Delta x^2}\\
&- D\frac{g^{n+1}_{i,j+1} - 2g^{n+1}_{i,j} + g^{n+1}_{i,j-1}}{\Delta y^2} = 0
\end{aligned} \tag{3.5}
$$

with the homogeneous boundary conditions of first kind

$$
g_{0,j} = g_{1,j} = g_{N_x,j} = g_{1,N_y} = 0 \tag{3.6}
$$

and the homogeneous initial condition

$$
g^0_{i,j} = p_{i,j} = p(x_i, y_j). \tag{3.7}
$$

4 Main Difference Equality

The fully implicite scheme described in section 4 allows to obtain a dicrete analogue of the integral equation (2.8) for the difference analogue (3.5) of the conjugate problem (2.6).

Let us consider a finite-difference approximation for equation (2.5):

$$u_n = \sum_{i,j} C_{i,j}^n \, p_{i,j}, \quad n = 0, 1, 2, ..., \tag{4.1}$$

where the summation is performed over all grid cells in the domain G. Assume that values of u_n are known. Find a relationship between source's components, z_n, and results of observations, u_n, in the same way as it was done in the continuous case.

Let $0 \leq k \leq n$. Taking the sum of the product $C_{i,j}^{n+1} g_{i,j}^{n-k}$ (see general notation (3.1)) over the grid $\omega_\tau \times \omega_h$, we obtain the following discrete equality:

$$\sum_{k=0}^{n-1} \sum_{i,j} z_k \, g_{i,j}^{n-k} \, \omega_{i,j} \, \Delta t = \sum_{i,j} (C_{i,j}^n \, p_{i,j} - g_{i,j}^n \, C_{i,j}^0). \tag{4.2}$$

Taking into account initial condition (2.3) ($C_{i,j}^0 = 0$) transform this equation into:

$$\sum_{i,j} K_{n-k} \, z_k = u_n, \quad n = 1, 2, ..., \tag{4.3}$$

where

$$K_n = \sum_{i,j} g_{i,j}^n \, \omega_{i,j} \, \Delta t. \tag{4.4}$$

We treat equation (4.3) as a system of linear equations to determine the unknown vector z_n. This system is a discrete analogue of the integral equation (2.8). In general it is ill-posed. A traditional method to solve such systems is Tikhonov's regularization. This technique prescribes finding the extremum of an α-parametrized smoothing functional. For the system of equations (4.3) this functional has the form

$$M^\alpha[z] = \sum_{n=0}^{N_t-1} (\sum_{k=0}^{n-1} (K_{n-k} \, z_k^\alpha - u_n)^2) + \alpha \, \Omega \, [z], \tag{4.5}$$

where

$$\Omega \, [z] = \sum_{n=0}^{N_\tau} [z_n^2 + (\Delta t)^{-2} (z_{n+1} - z_n)^2] \tag{4.6}$$

is a stabilizing functional.

A choice of a regularization parameter α is often based on the principle of residual (see Morozov, 1968) that defines α to be a solution of the equation

$$\sum_{n=0}^{N_t-1} (\sum_{k=0}^{n-1} (K_{n-k} \, z_k^\alpha - u_{\delta,n})^2 = \delta^2, \tag{4.7}$$

where

$$u_\delta = (u_{\delta,0}, u_{\delta,1}, ..., u_{\delta,N_t-1}) \tag{4.8}$$

is a vector obtained from observations whose average square error is estimated by δ:

$$\sum_{n=0}^{N_\tau-1} (u_{\delta,n} - u_n)^2 \leq \delta^2. \tag{4.9}$$

It is shown (Morozov, 1968) that this algorithm of approximate solution is a regularization technique, i.e. it ensures the convergence of corresponding approximations to the exact solution as $\delta \to 0$.

5 The Results of Testing

For testing the algorithm, a series of calculations with different values of the regularization parameter α, different accuracies of observation results $u(t)$, and different numbers of time steps N_t have been performed. Different types of source's time component $z(t)$ have been tested. Here we present some results of simulation and compare them with the exact solutions. The first series of simulations has been performed for the source function $z(t) = sin(t)$ with a 5% error in u. An error was introduced as a sign-changing addition to function u with absolute value 5% of u. The number of time steps is $N_t = 32$.

Figure 1 shows the results of calculations for $\alpha = 0$. The exact solution is shown by asterisks $*$ and the results of reconstruction by the dashed line $--$. As one can see on the Figure 1 there is no sufficient reconstruction.

Figures 2-5 show the results of calculations for the values of $\alpha: 10^{-9}, 10^{-8}, 10^{-7}, 10^{-6}$ respectively. The best results are obtained for $\alpha = 10^{-7}$.

In **Table 1** the square of the norm of the difference between exact and reconstructed solutions, the square of the norm of the difference between exact and approximated right-hand sides and the square of the norm of the residual for equation (4.3) on the reconstructed solution are given for different values of α. The best results are obtained for the residual norm slightly greater than the error in the right-hand side. Notice that on the last times steps the reconstruction is not good enough. This fact is, probably, caused by the contamination propagation delay.

Figure 6 shows how the kernel of equation (4.3) depends on time. The delay in the contaminant propagation is approximately equal to the period of time, during which the kernel reaches its maximum value. Therefore the reconstruction of the source is not accurate if this period exceeds the period of observation.

Figures 7-9 show the results of calculations for the same parameters, with a 1% error in the right-hand side u. The error has been modeled as a sign-changing addition to the right-hand side.

Table 2 shows the same values as **Table 1**. As it was expected the accuracy of reconstruction increases, but a time period, mentioned in the previous paragraph, still exists.

Figures 10-14 and **Table 3** show the results of calculations for the same parameters, with the number of time steps $N_t = 64$. Increasing a number of time steps does not strongly improve the result of reconstruction and the number of unsatisfactorily reconstructed points at the end of the time period.

Figures 15-18 and **Table 4** show the results of simulations for the discontinuous source function

$$z(t) = \begin{cases} 1 & \text{if } 0 \leq t < 0.4, \\ 2 & \text{if } 0.4 \leq t < 0.625, \\ 1 & \text{if } t \geq 0.625. \end{cases}$$

Notice that in the discontinuity region the reconstructed solution is spreaded and the width of spreading is approximately equal to the time delay of the contamination propagation.

Figures 19-22 and **Table 5** show the results of simulations for another discontinuous source function:

$$z(t) = \begin{cases} 1 & \text{if } 0 \leq t < 0.25, \\ 2 & \text{if } 0.25 \leq t < 0.5, \\ 0 & \text{if } 0.5 \leq t < 0.625, \\ 3 & \text{if } 0.625 \leq t < 0.85, \\ 1 & \text{if } t \geq 0.85. \end{cases}$$

In this case satisfactory reconstruction is also obtained.

α	$\|z^\alpha - z\|^2$	$\|u_\delta - u\|^2$	$\|Kz^\alpha - u\|^2$
0	$1.011 \cdot 10^2$	$1.428 \cdot 10^{-8}$	$7.656 \cdot 10^{-32}$
10^{-9}	$1.507 \cdot 10^0$	$1.428 \cdot 10^{-8}$	$1.085 \cdot 10^{-8}$
10^{-8}	$1.833 \cdot 10^{-2}$	$1.428 \cdot 10^{-8}$	$1.393 \cdot 10^{-8}$
10^{-7}	$1.815 \cdot 10^{-2}$	$1.428 \cdot 10^{-8}$	$1.594 \cdot 10^{-8}$
10^{-6}	$5.262 \cdot 10^{-2}$	$1.428 \cdot 10^{-8}$	$5.418 \cdot 10^{-8}$

Table 1 $(\Delta = 0.05, \; N_t = 32, \; z(t) = sin(t))$.

α	$\|z^\alpha - z\|^2$	$\|u_\delta - u\|^2$	$\|Kz^\alpha - u\|^2$
0	10^2	10^{-8}	10^{-32}
10^{-9}	$5.64 \cdot 10^{-2}$	$5.70 \cdot 10^{-10}$	$4.42 \cdot 10^{-10}$
10^{-8}	$7.13 \cdot 10^{-3}$	$5.70 \cdot 10^{-10}$	$6.34 \cdot 10^{-10}$
10^{-7}	$2.09 \cdot 10^{-2}$	$5.70 \cdot 10^{-10}$	$6.34 \cdot 10^{-10}$
10^{-6}	$5.35 \cdot 10^{-2}$	$5.70 \cdot 10^{-10}$	$2.04 \cdot 10^{-9}$

Table 2 $(\delta = 0.01, \; N_t = 32, \; z(t) = sin(t))$.

α	$\|z^\alpha - z\|^2$	$\|u_\delta - u\|^2$	$\|Kz^\alpha - u\|^2$
0	$\cdot 10^2$	$\cdot 10^{-8}$	$\cdot 10^{-32}$
10^{-9}	$4.23 \cdot 10^{-2}$	$3.64 \cdot 10^{-10}$	$2.82 \cdot 10^{-10}$
10^{-8}	$8.33 \cdot 10^{-3}$	$3.64 \cdot 10^{-10}$	$4.05 \cdot 10^{-10}$
10^{-7}	$1.87 \cdot 10^{-2}$	$3.64 \cdot 10^{-10}$	$2.06 \cdot 10^{-9}$
10^{-6}	$5.54 \cdot 10^{-2}$	$3.64 \cdot 10^{-10}$	$6.50 \cdot 10^{-8}$

Table 3 $(\Delta = 0.01, \; N_\tau = 64 \; z(t) = sin(t))$.

α	$\|z^\alpha - z\|^2$	$\|u_\delta - u\|^2$	$\|Kz^\alpha - u\|^2$
0	$\cdot 10^2$	$\cdot 10^{-8}$	$\cdot 10^{-32}$
10^{-9}	$6.50 \cdot 10^{-1}$	$6.00 \cdot 10^{-9}$	$4.55 \cdot 10^{-9}$
10^{-8}	$2.86 \cdot 10^{-2}$	$6.00 \cdot 10^{-9}$	$5.80 \cdot 10^{-9}$
10^{-7}	$3.33 \cdot 10^{-2}$	$6.00 \cdot 10^{-9}$	$7.64 \cdot 10^{-8}$
10^{-6}	$6.94 \cdot 10^{-2}$	$6.00 \cdot 10^{-9}$	$7.34 \cdot 10^{-8}$

Table 4 ($\delta = 0.01, \quad N_t = 64$)

α	$\|z^\alpha - z\|^2$	$\|u_\delta - u\|^2$	$\|Kz^\alpha - u\|^2$
0	$\cdot 10^2$	$\cdot 10^{-8}$	$\cdot 10^{-32}$
10^{-9}	$1.02 \cdot 10^{0}$	$9.19 \cdot 10^{-9}$	$6.92 \cdot 10^{-9}$
10^{-8}	$8.99 \cdot 10^{-2}$	$9.19 \cdot 10^{-9}$	$9.04 \cdot 10^{-9}$
10^{-7}	$1.36 \cdot 10^{-1}$	$9.19 \cdot 10^{-9}$	$1.65 \cdot 10^{-8}$
10^{-6}	$3.00 \cdot 10^{-1}$	$9.19 \cdot 10^{-9}$	$2.54 \cdot 10^{-7}$

Table 5 ($\delta = 0.01, \quad N_t = 64$)

Acknowledgement
The authors thank Dr. A. Kryazhimskii for useful discussions.

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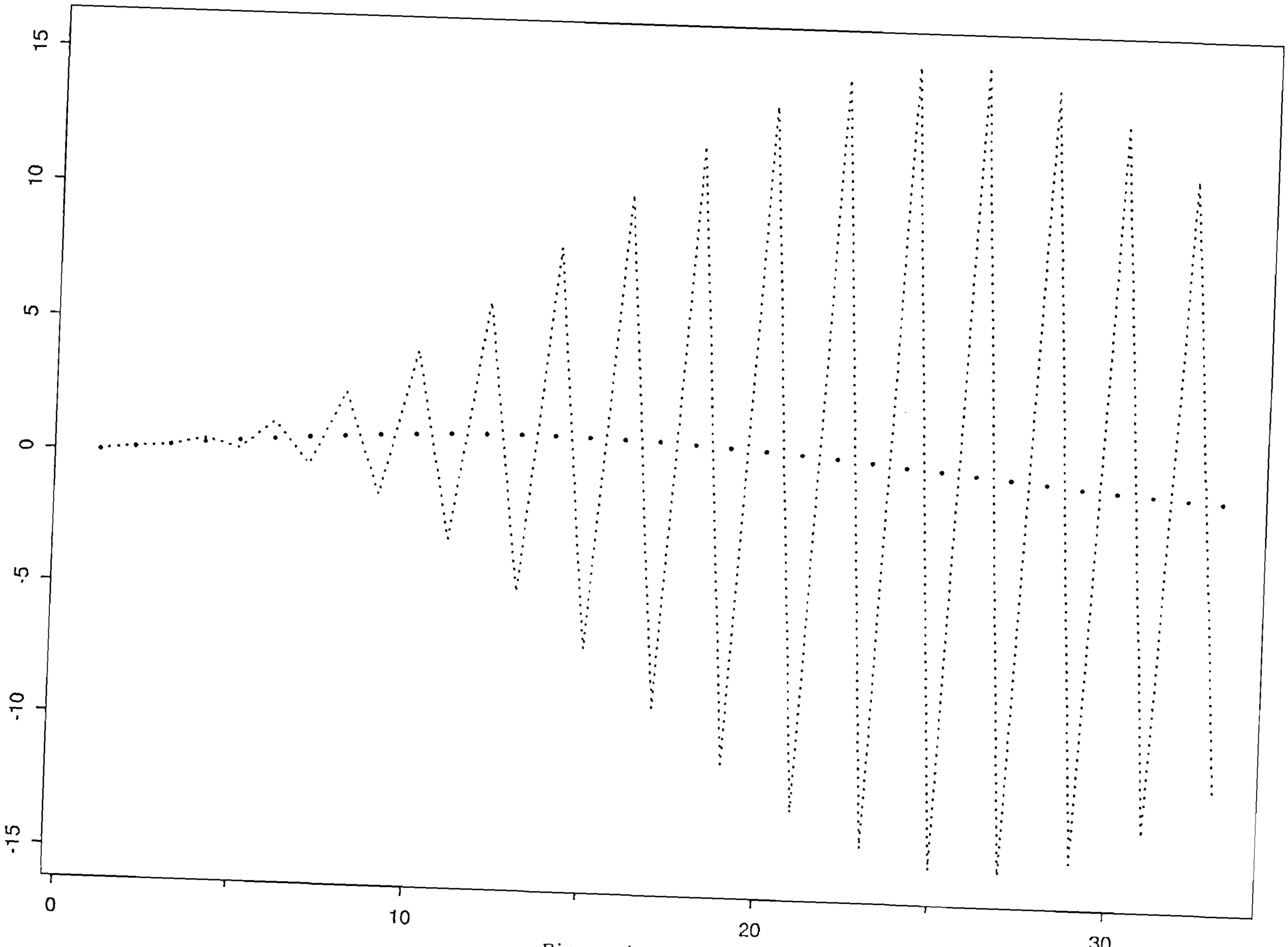


Figure 1

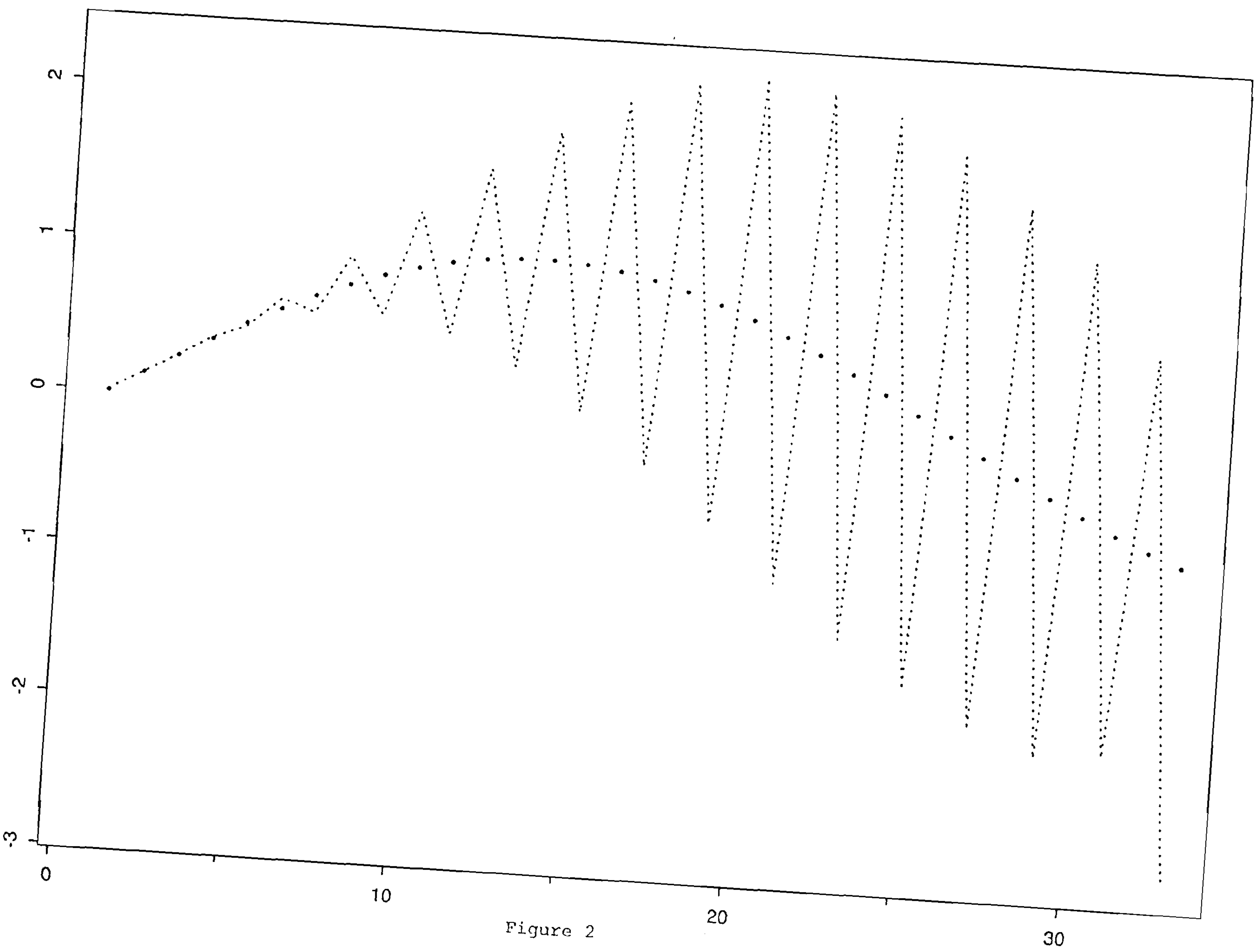


Figure 2

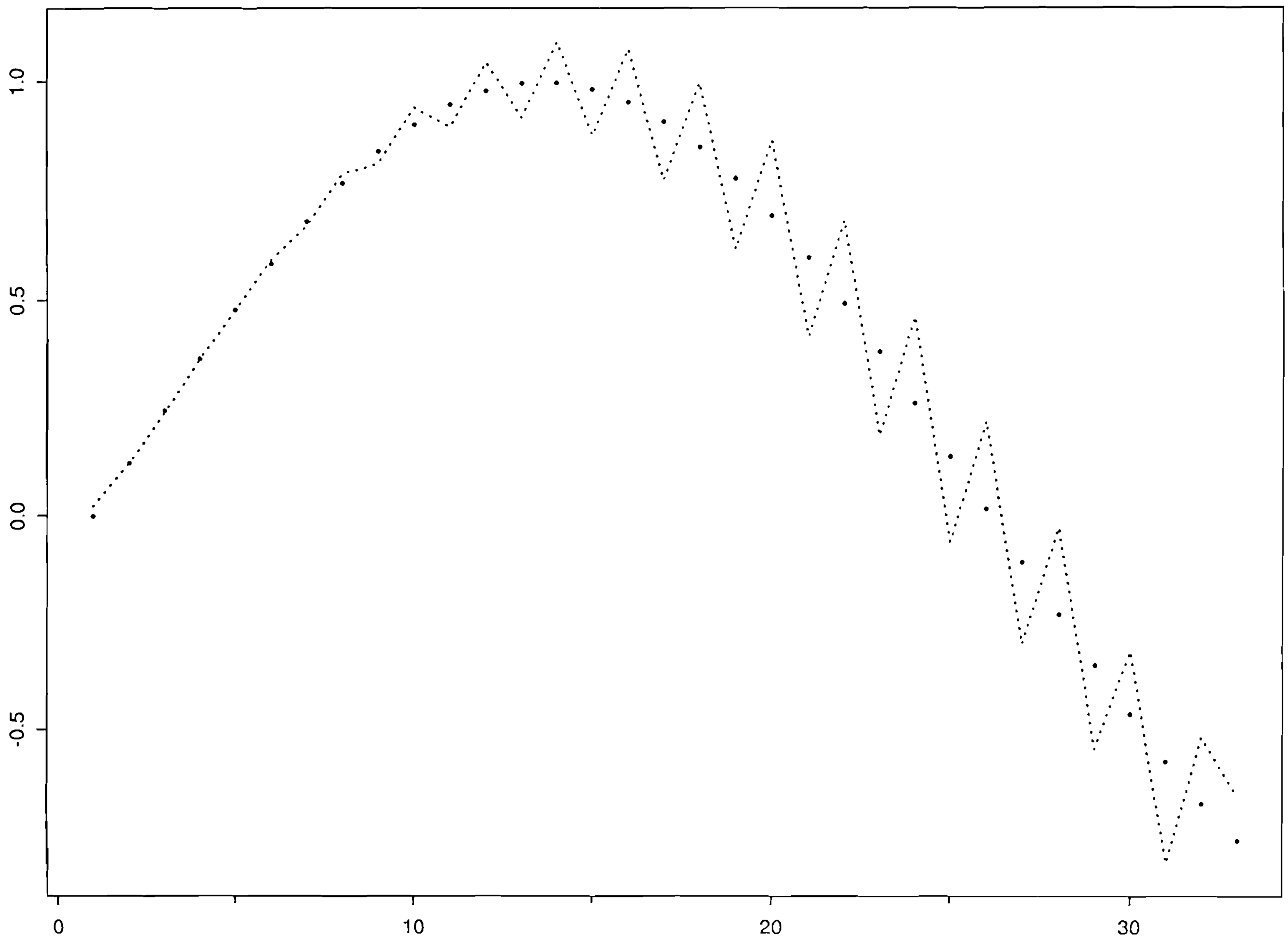


Figure 3

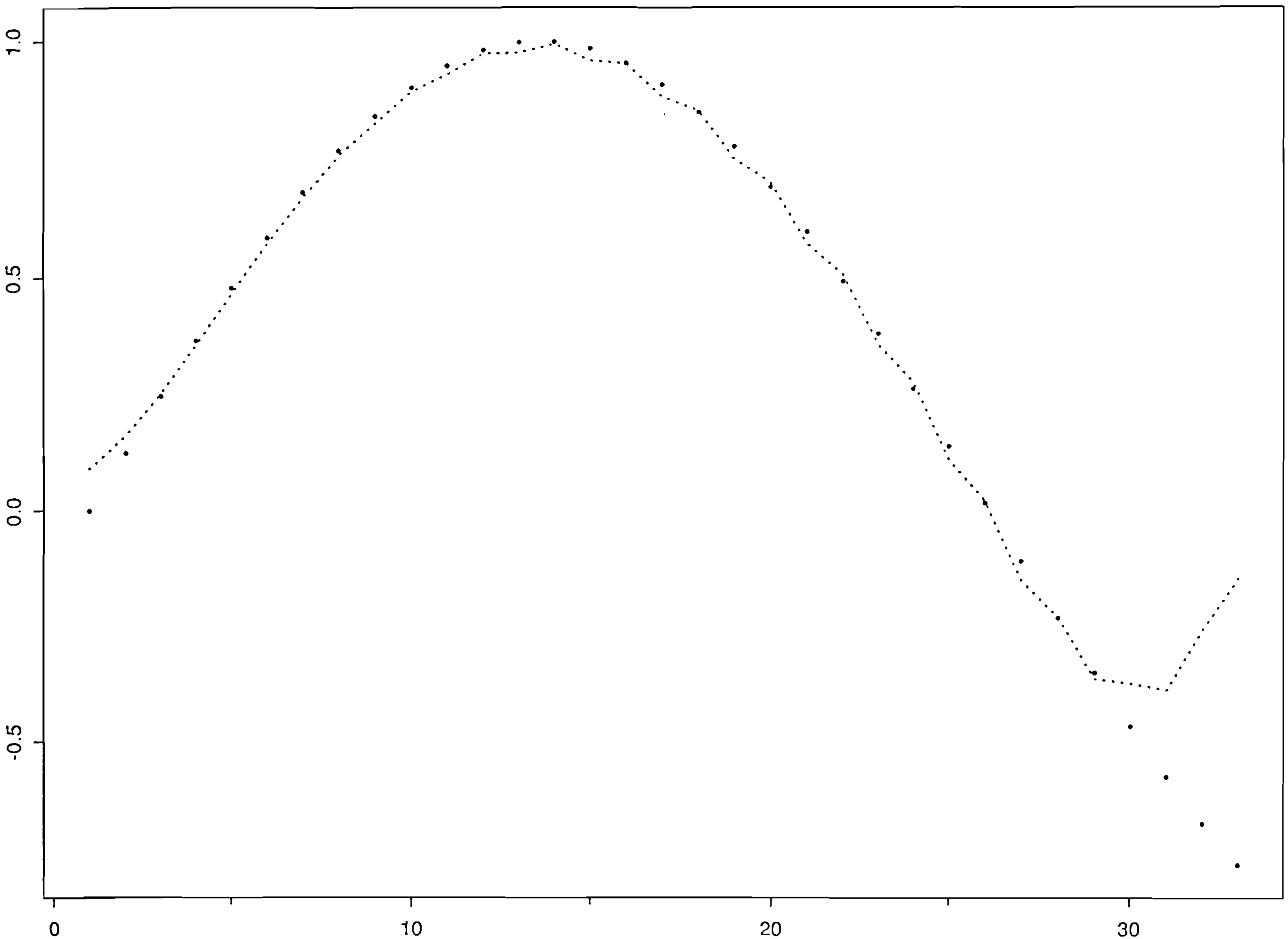
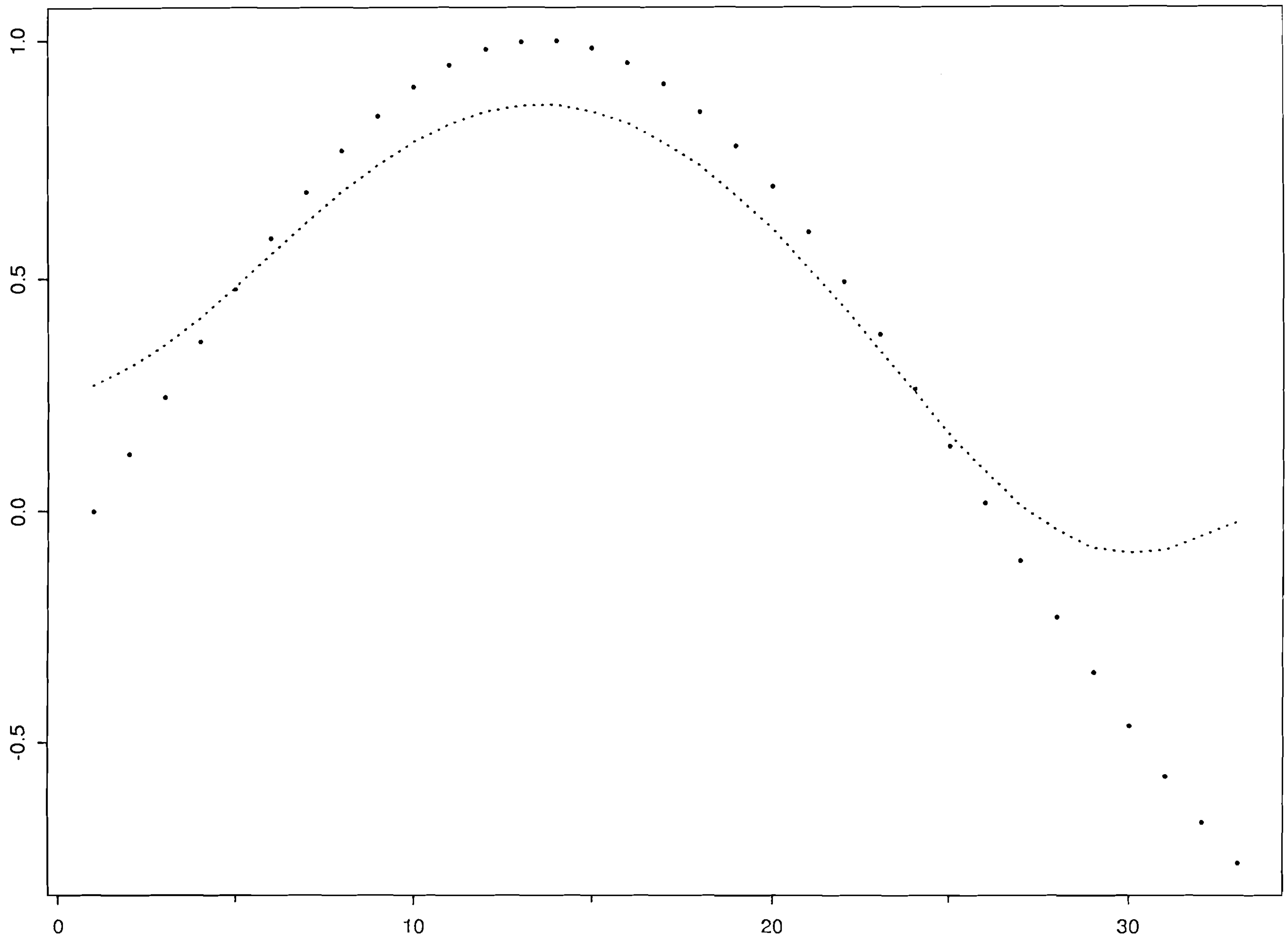


Figure 4



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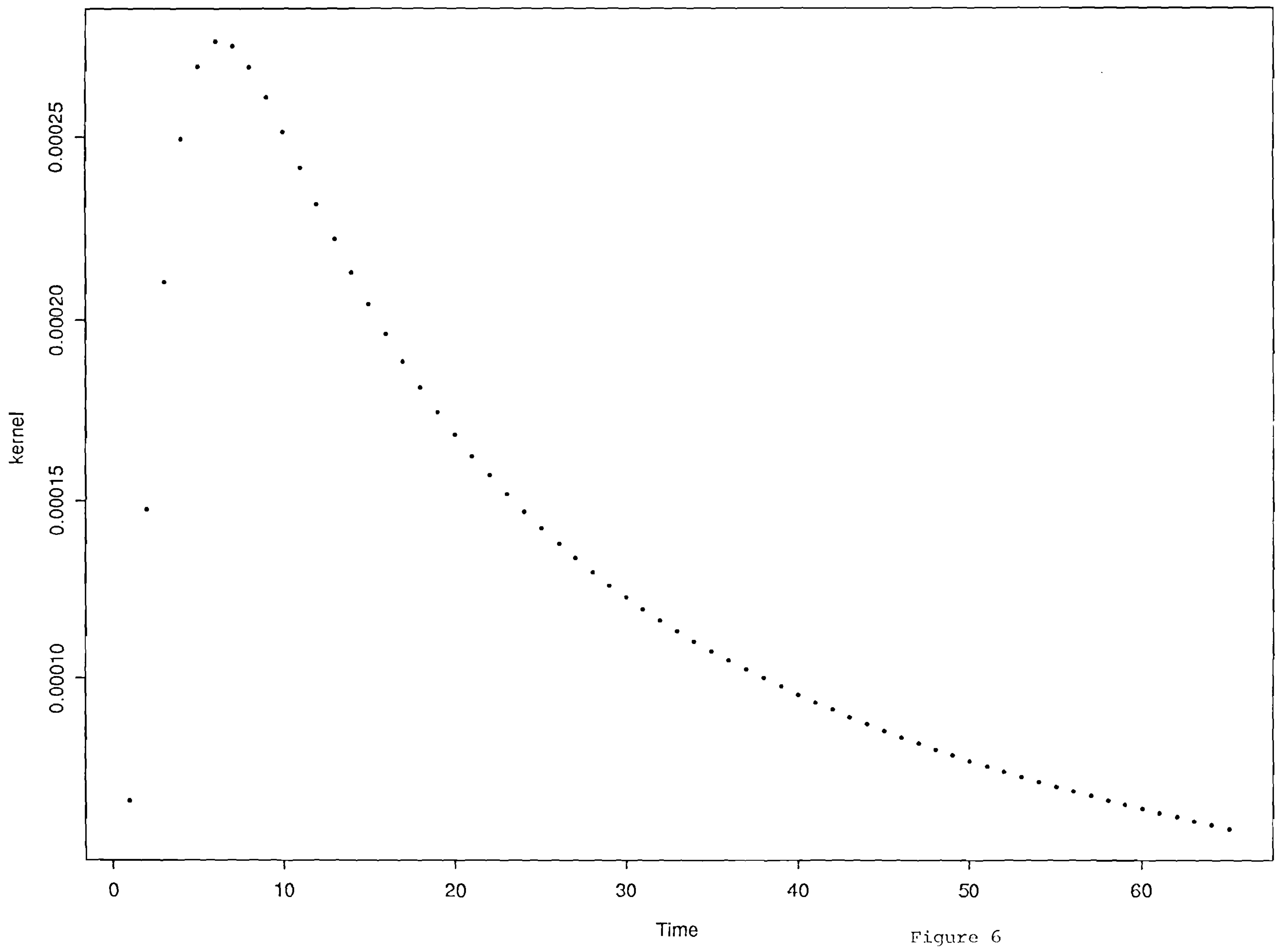


Figure 6

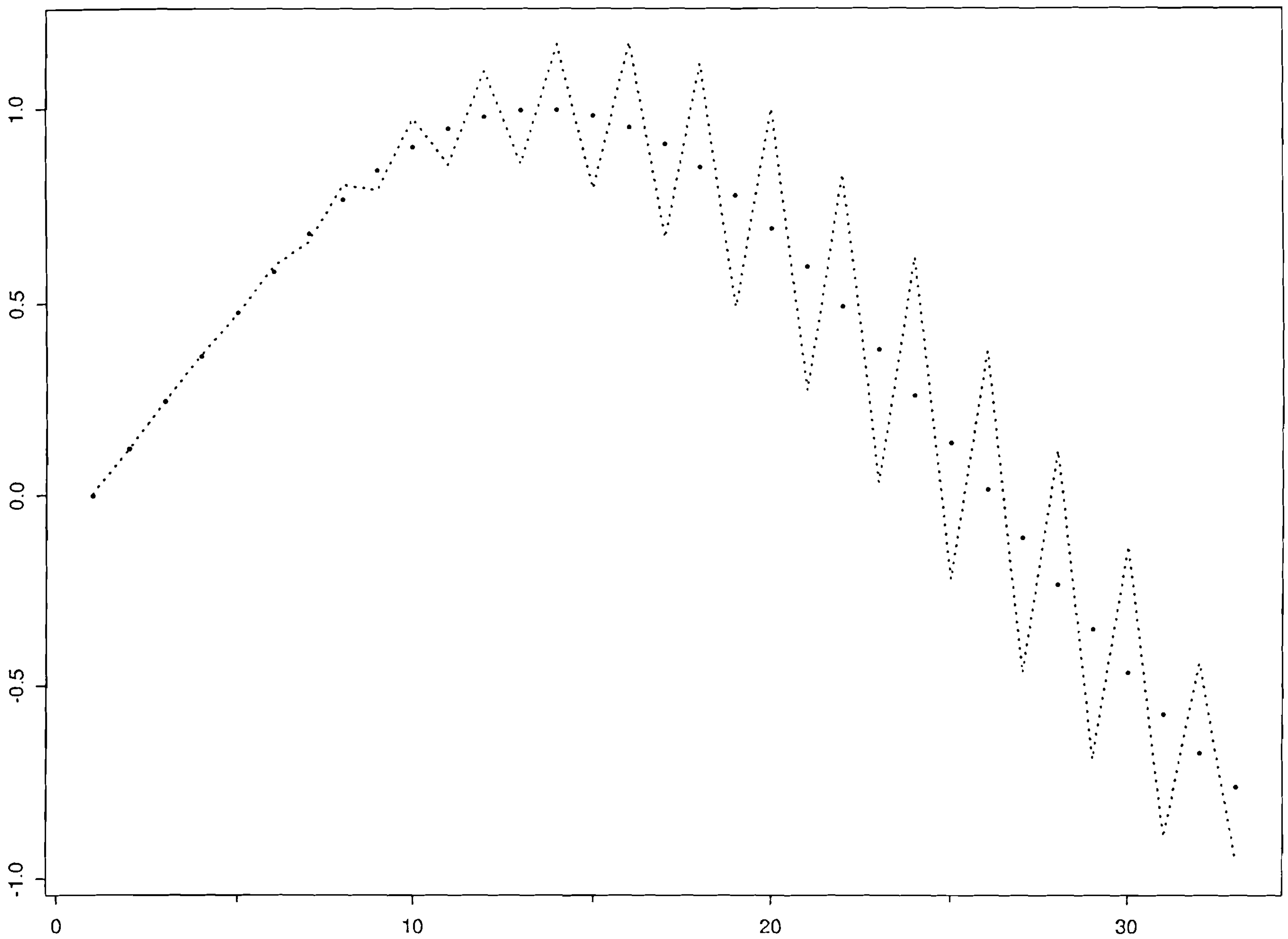
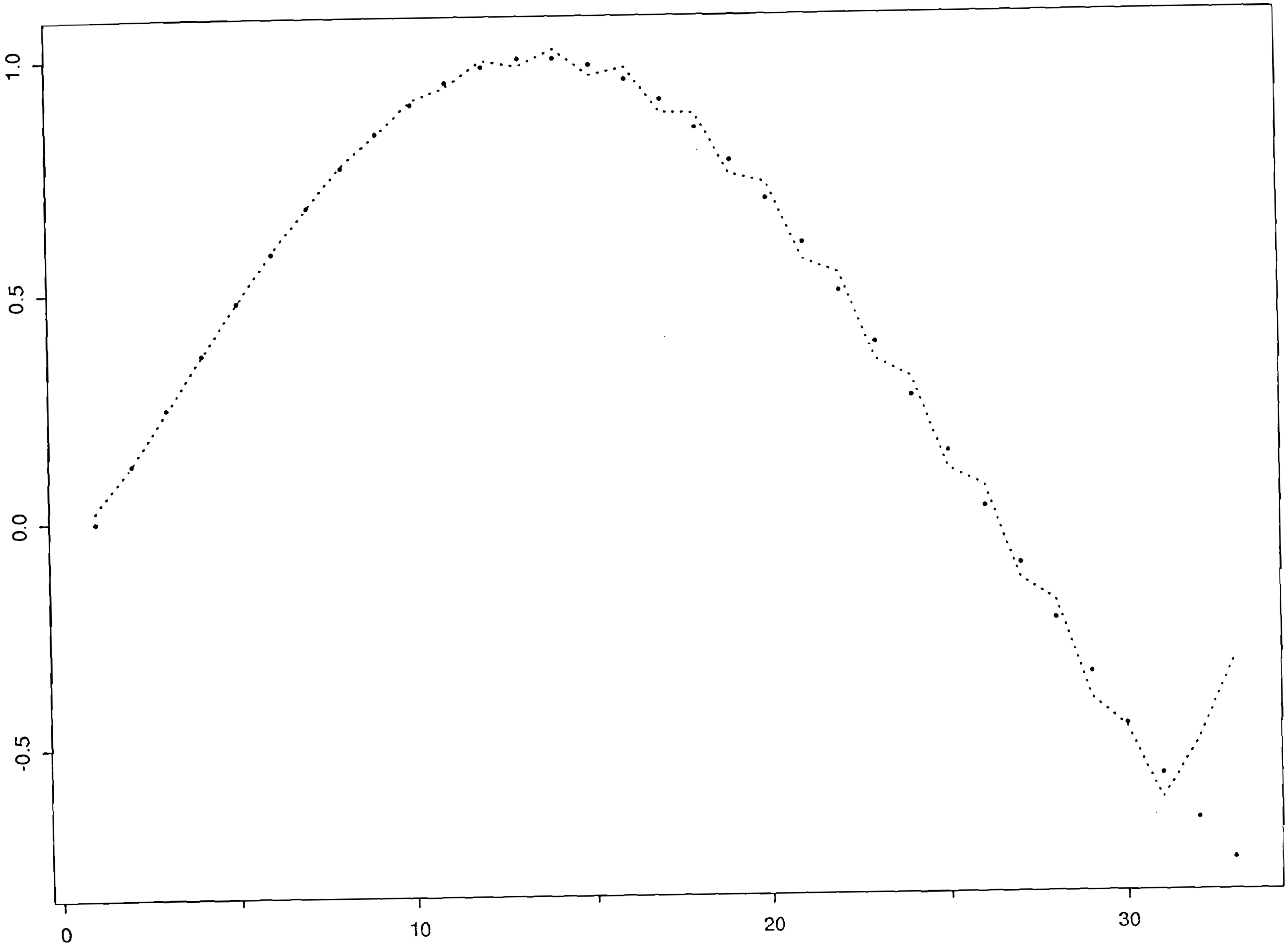


Figure 7



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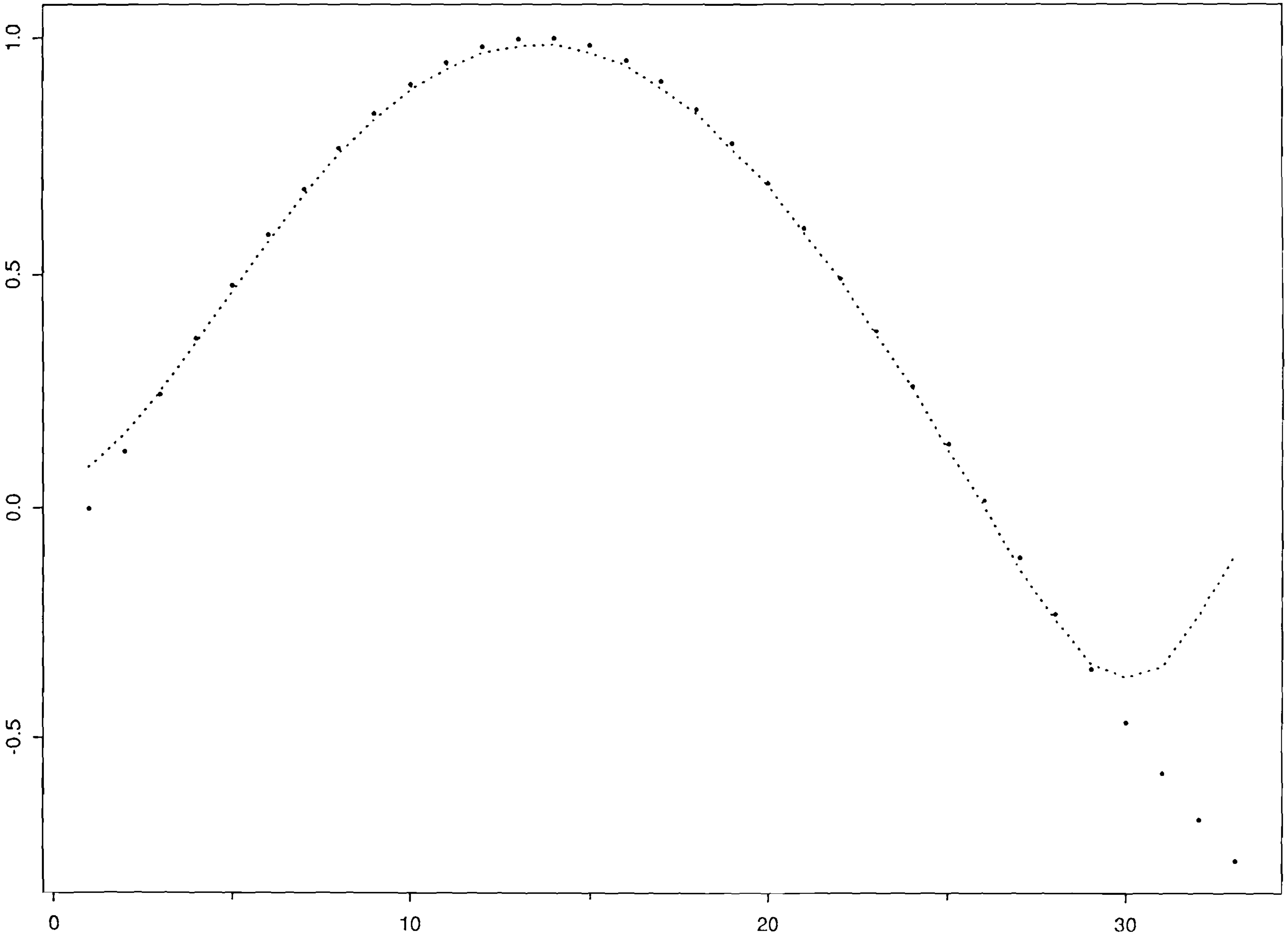

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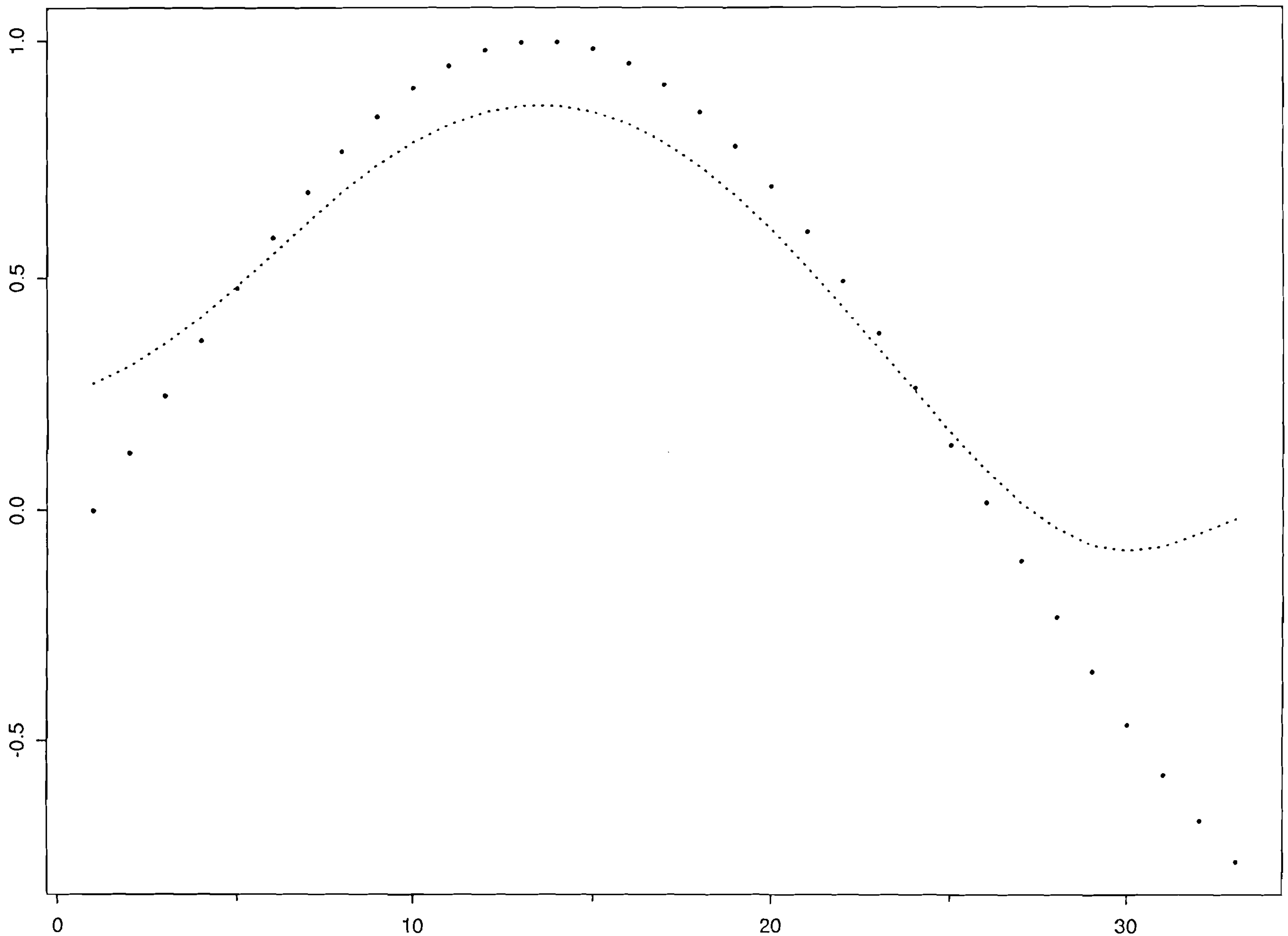

Figure 10

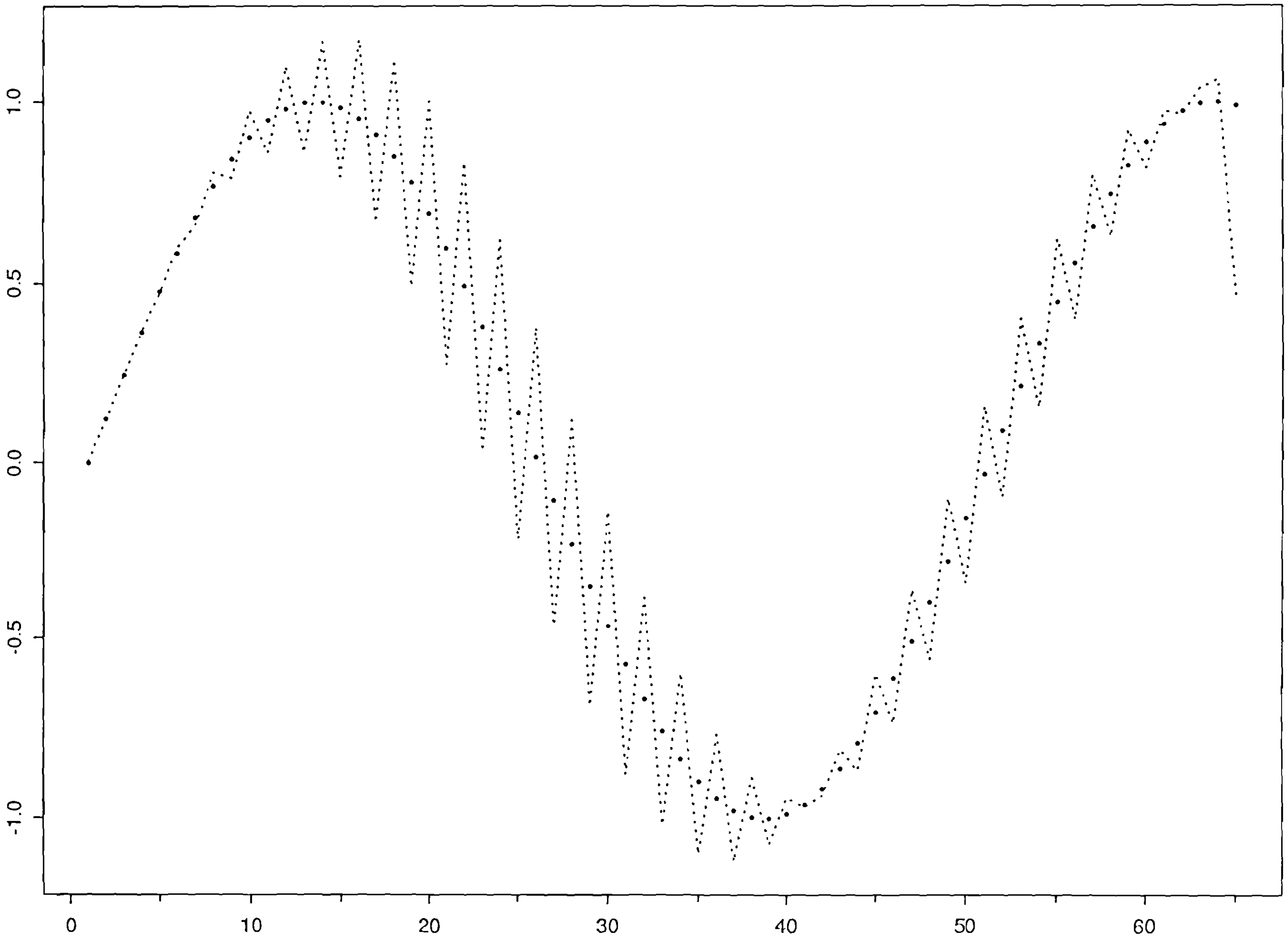

Figure 11

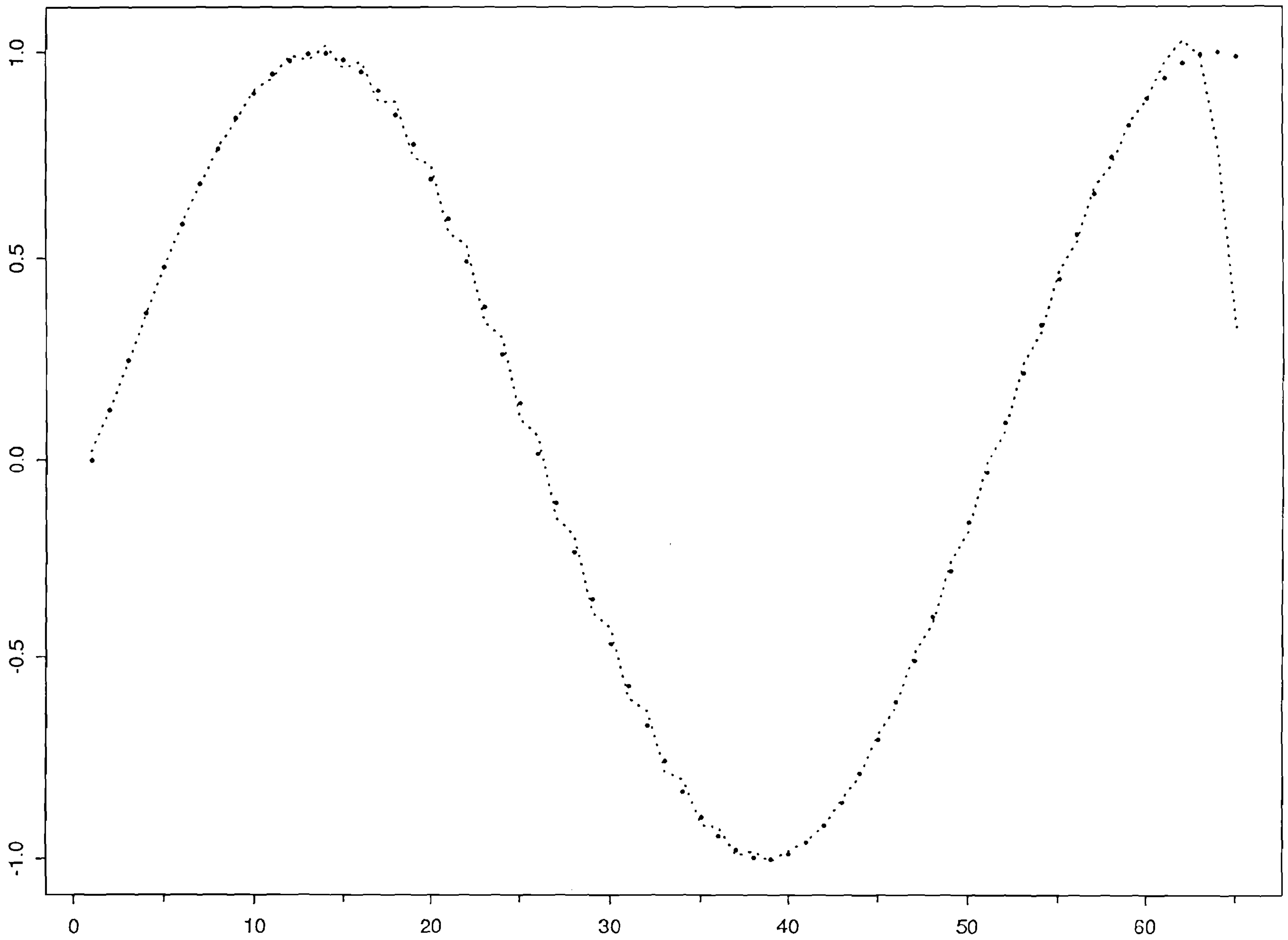

Figure 12

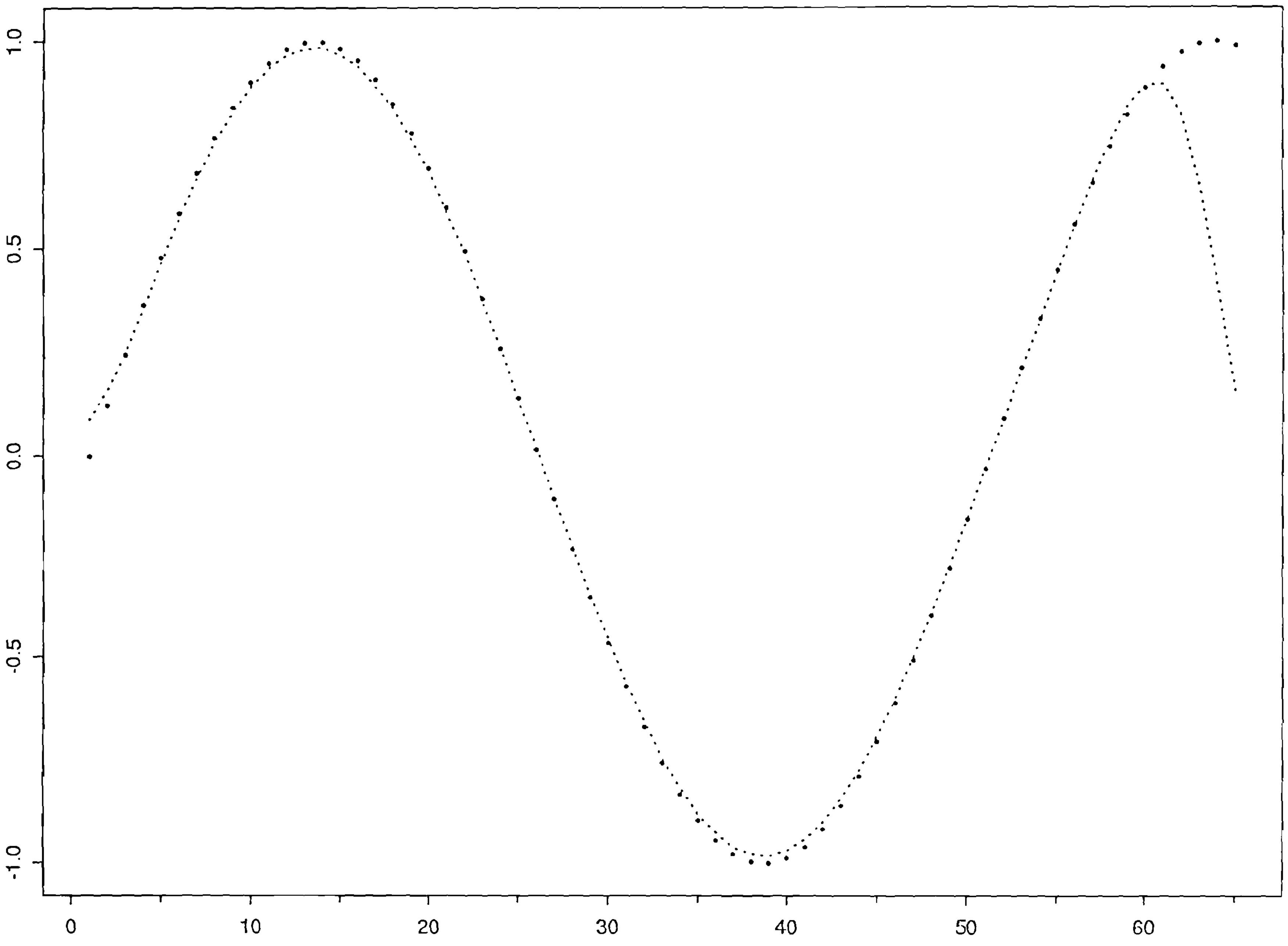

Figure 13

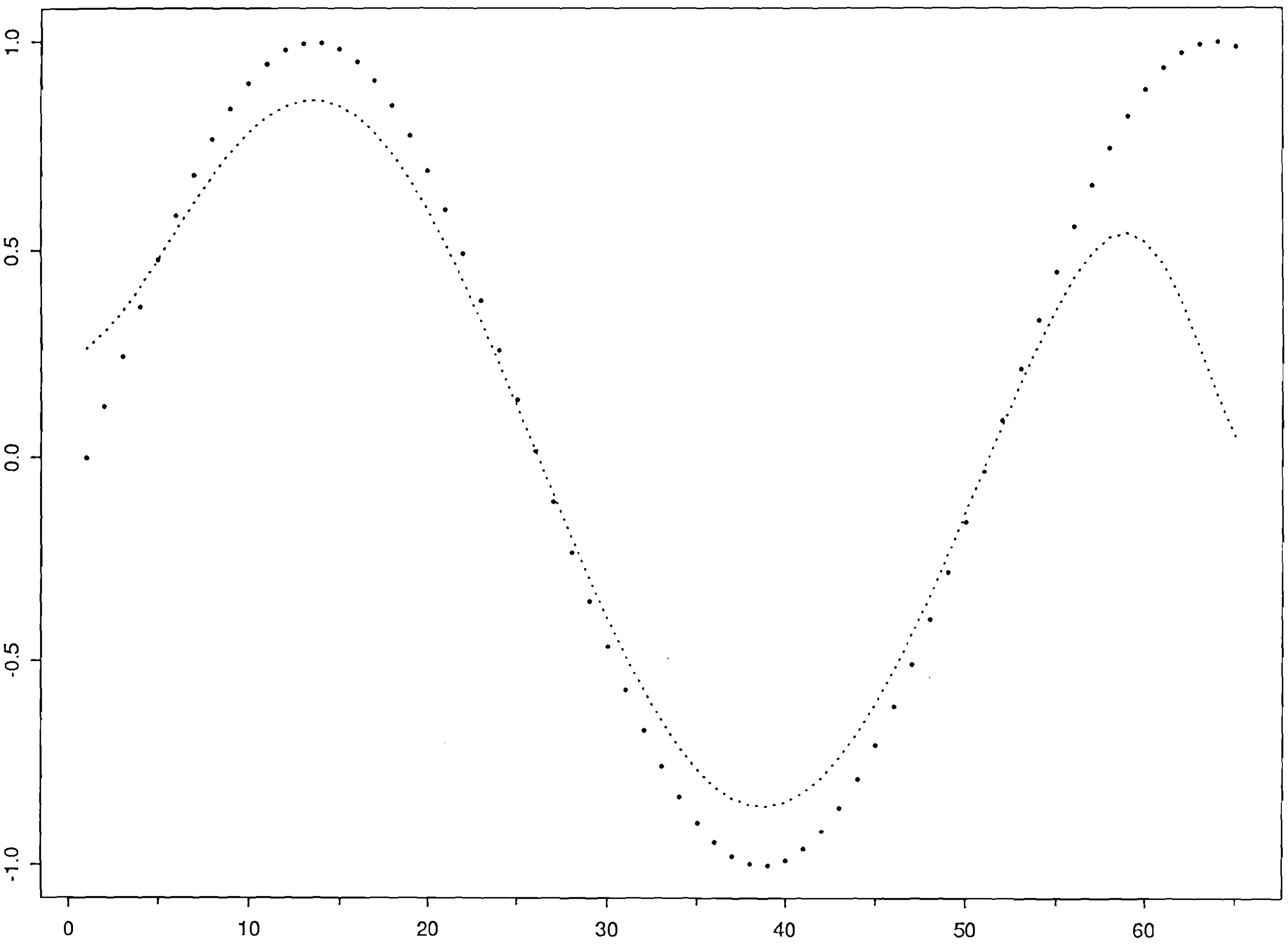

Figure 14

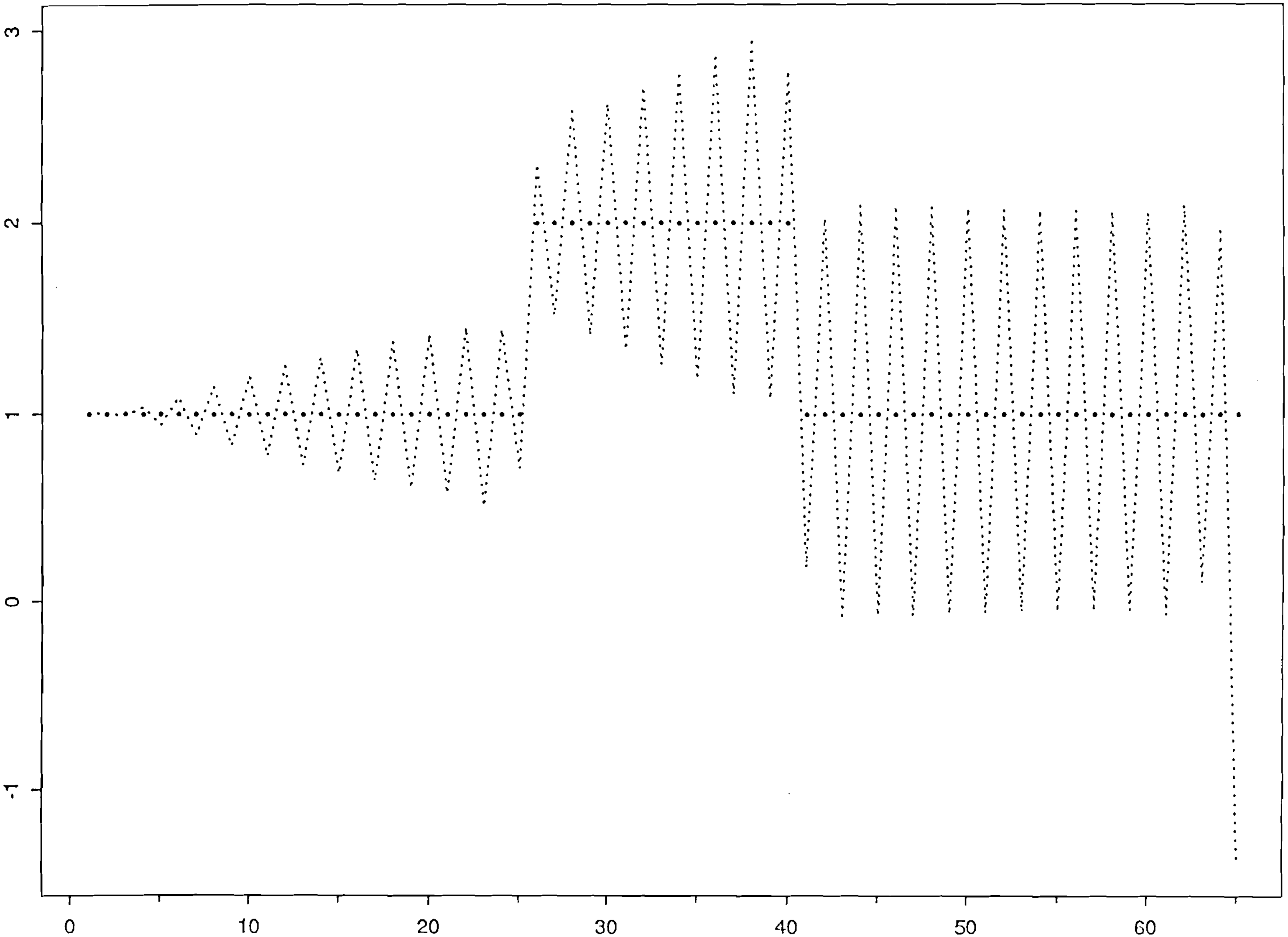

Figure 15

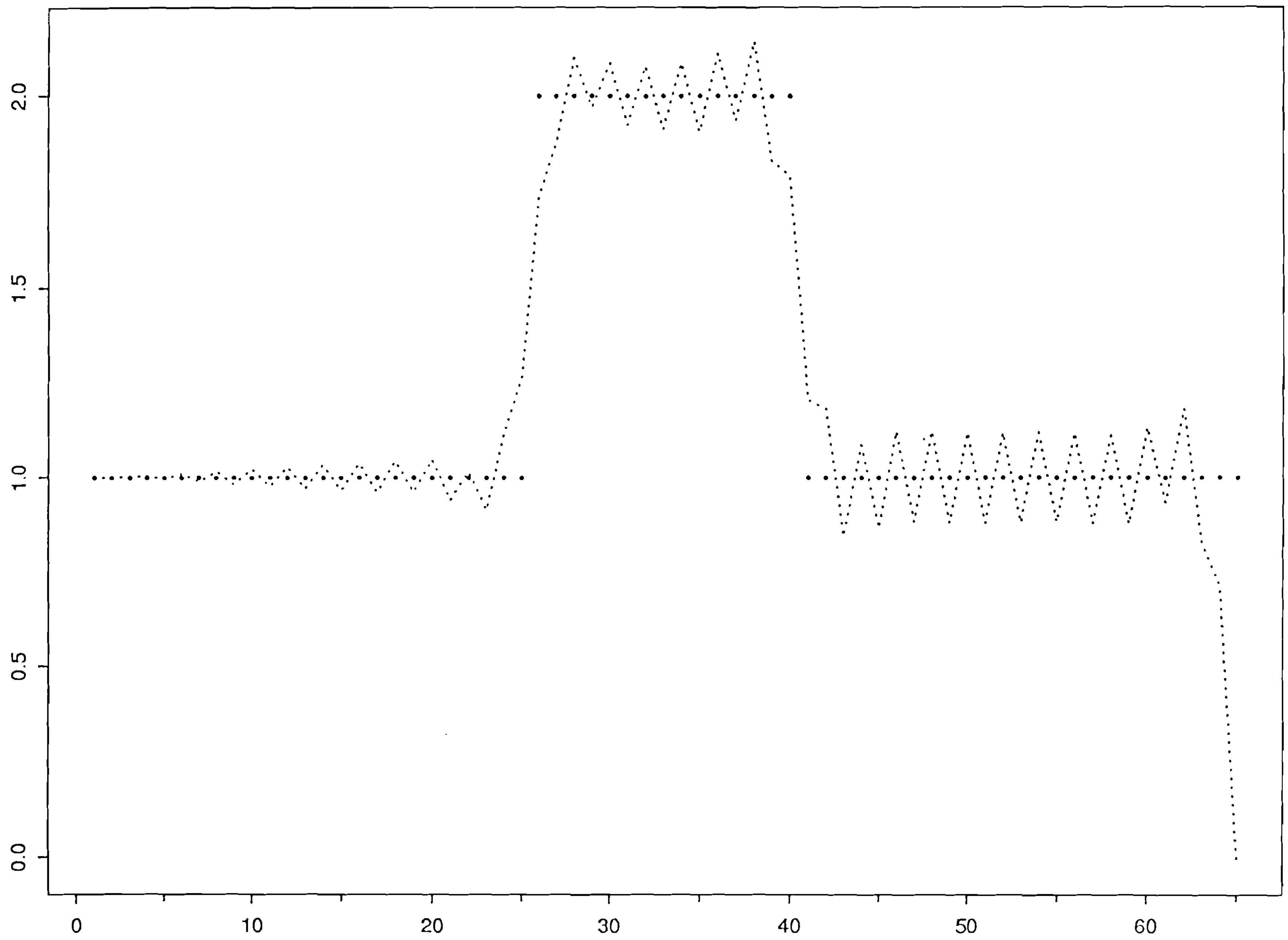

Figure 16

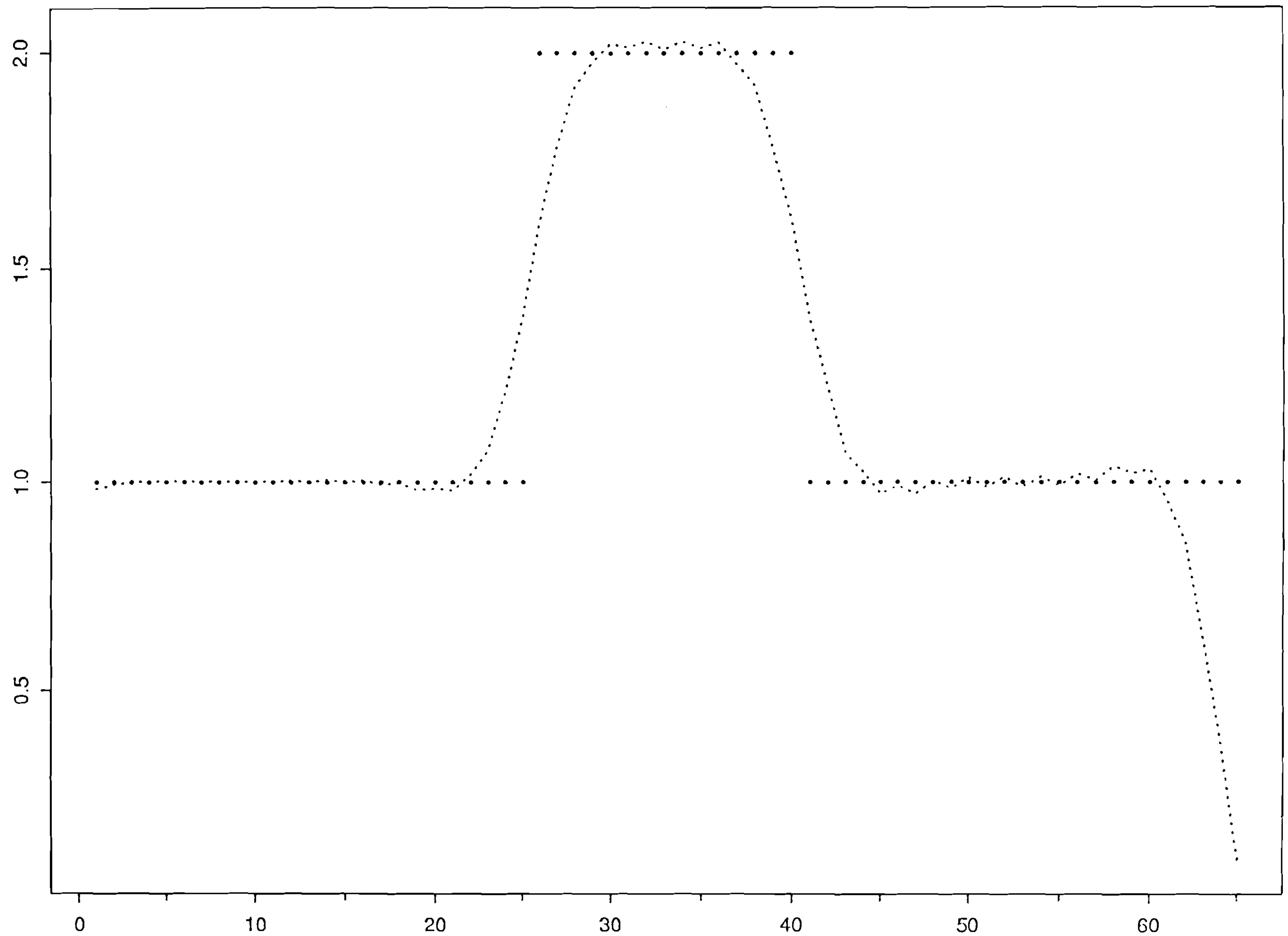

Figure 17

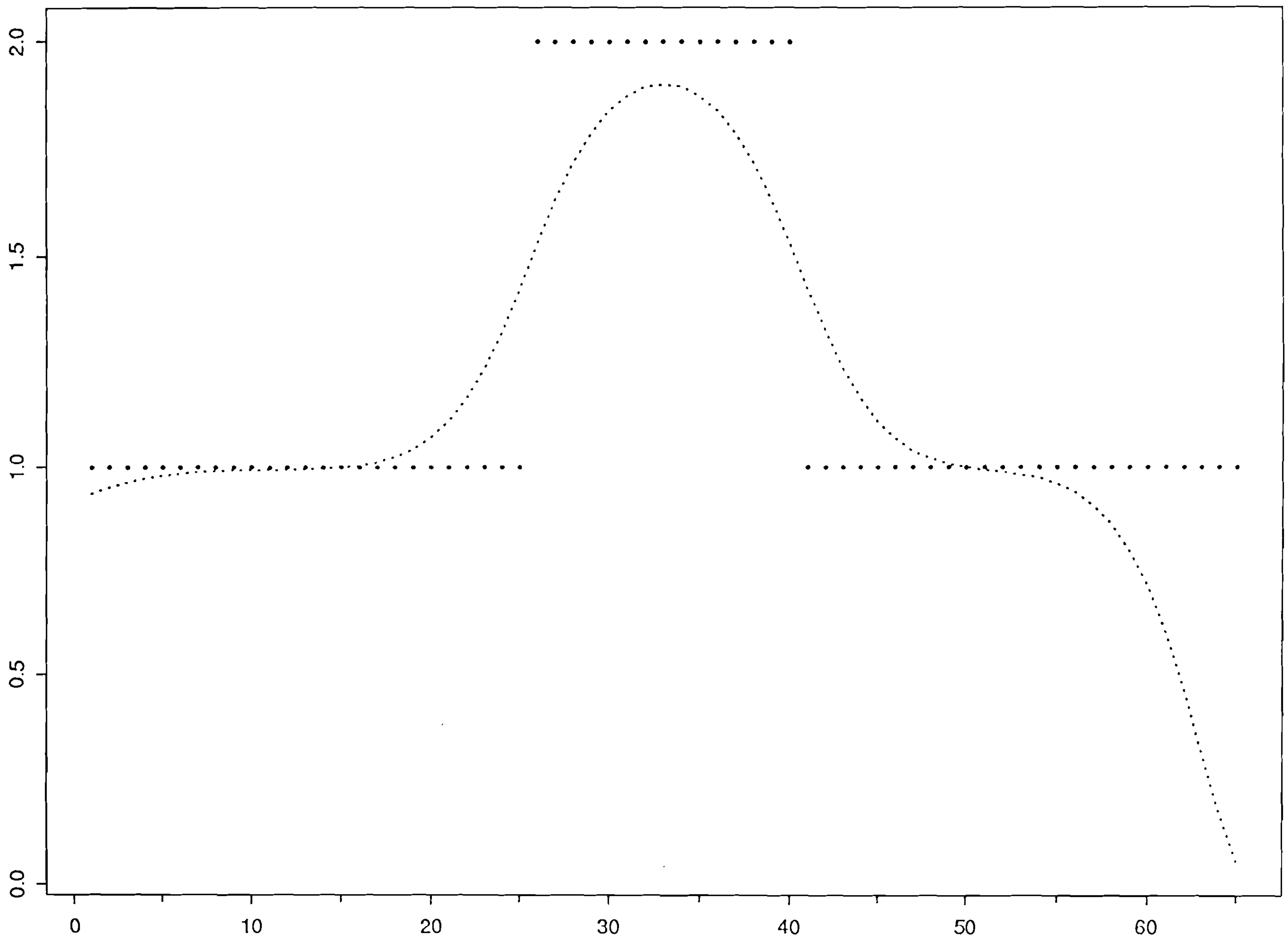

Figure 18

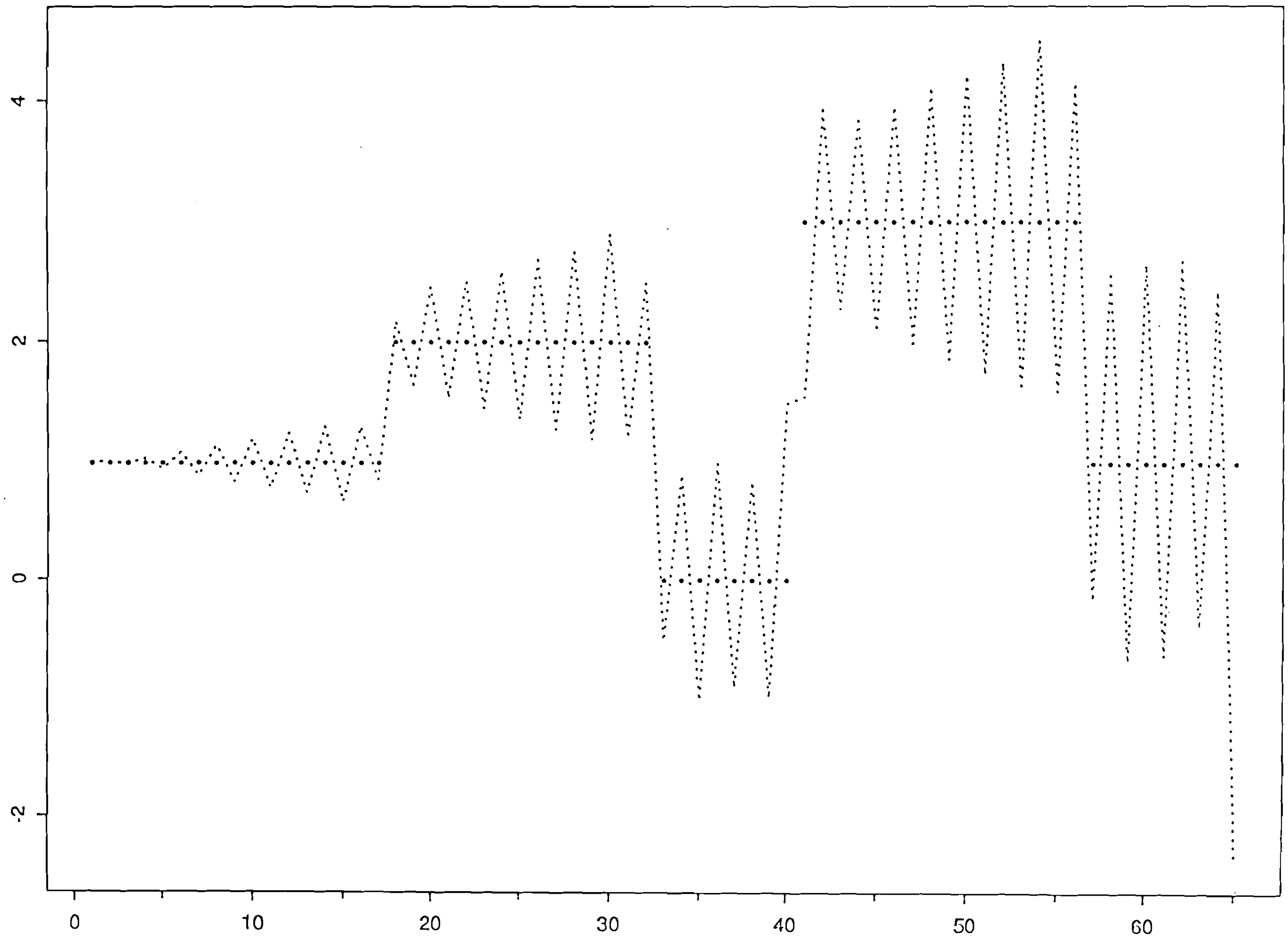

Figure 19

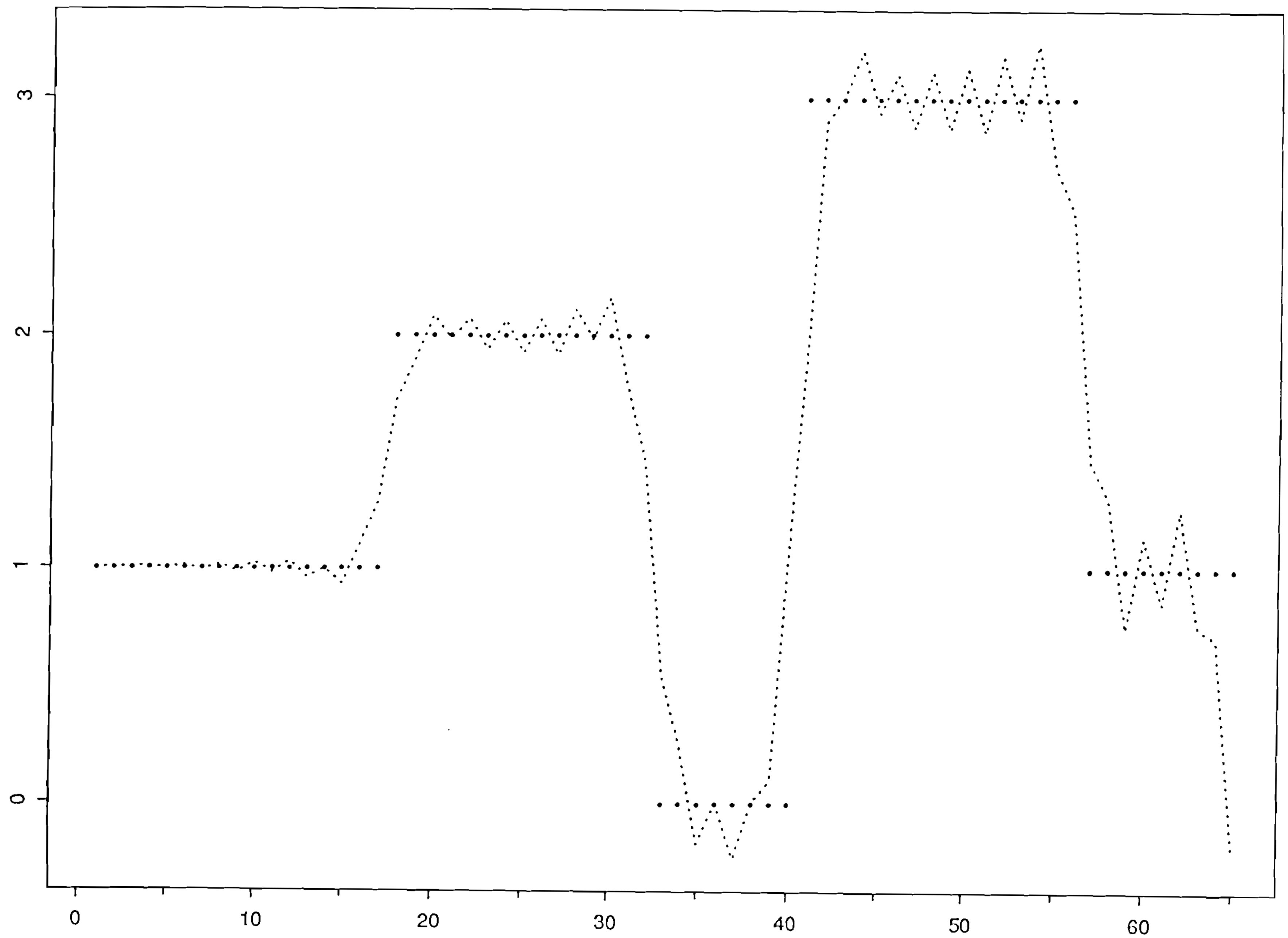

Figure 20

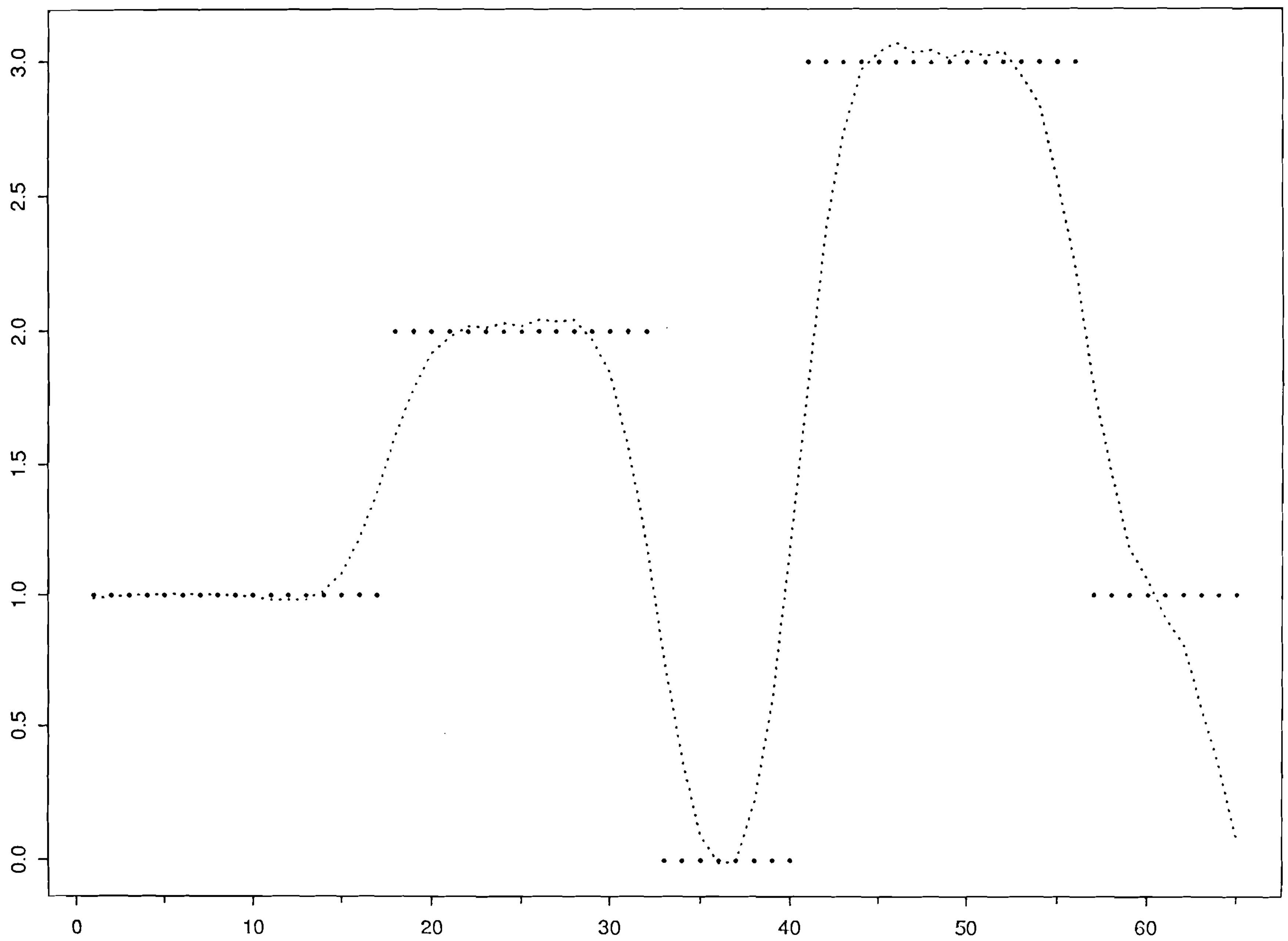

Figure 21

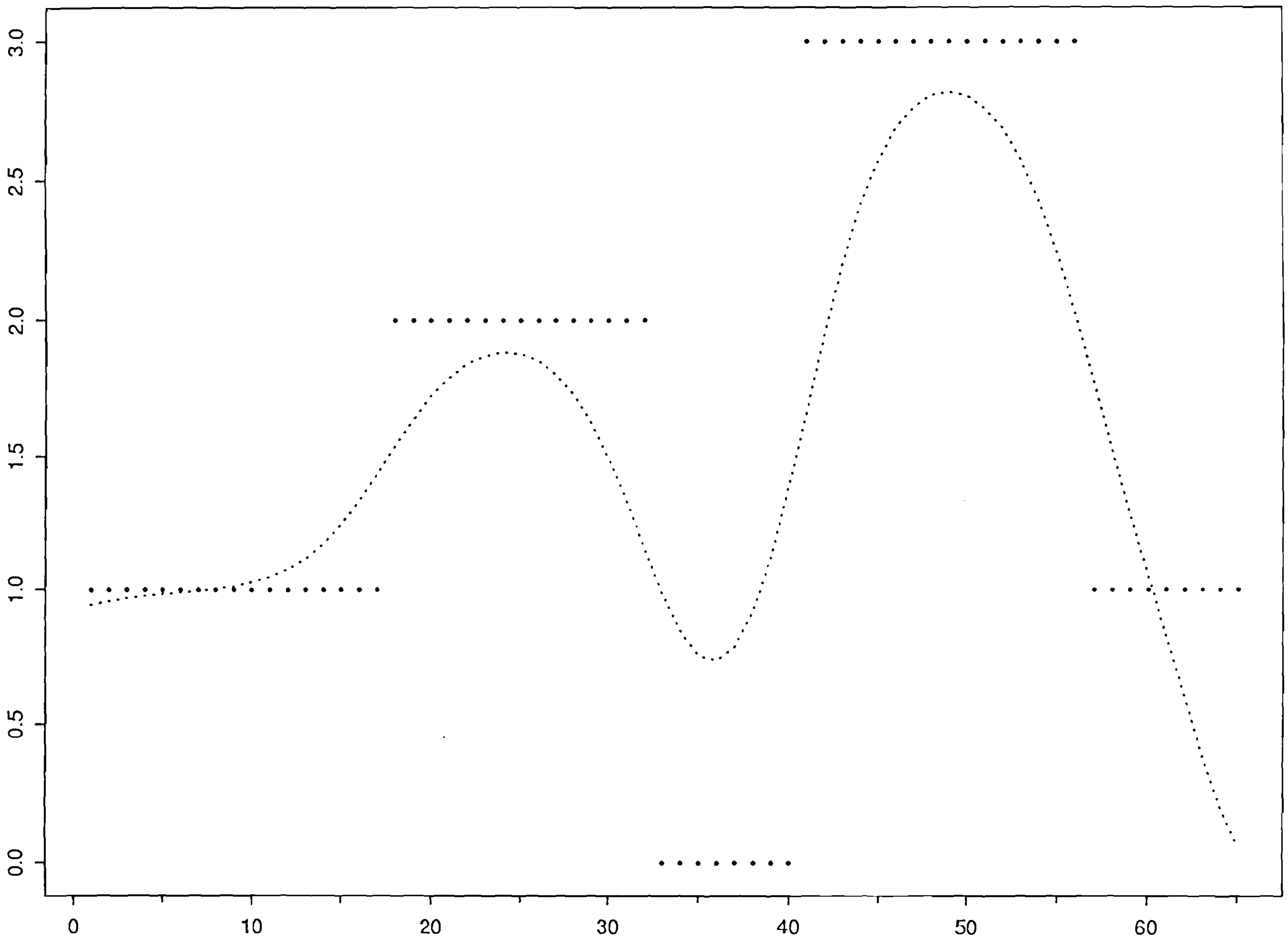

Figure 22