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Publication date: 1983

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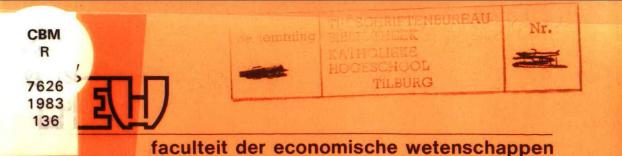
Citation for published version (APA): Kleijnen, J. P. C. (1983). *On the interpretation of variables*. (Research memorandum / Tilburg University, Department of Economics; Vol. FEW 136). Unknown Publisher.

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RESEARCH MEMORANDUM





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ON THE INTERPRETATION OF VARIABLES

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October 1983

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CONTENTS

Abstract	v
1. Introduction	1
2. Types of variables	1
3. Measurement scales and regression	6
4. User view: risk and sensitivity analysis	10
5. User view: optimization and what-if	15
6. Summary	16
Appendix 1: Coding of variables	17
" 2: Risk analysis on regression models	18

11	3:	Inverse	regression	in	control	problems	23

References

ABSTRACT

The input of a computer program, say a simulation program, specifies parameters, variables, and behavioral relationships. Parameters are not directly observable. Variables can be specified through enumeration, mathematical functions, and scenarios. In regression models the scenarios correspond to binary variables. Regression models accept different measurement scales: nominal, interval, ratio, absolute scales. The interpretation of interval variables may be misleading if there are interactions between regression variables. The interpretation of quantitative and qualitative variables (in regression versus ANOVA models) is different. The user distinguishes between environmental and controllable variables. Environmental variables involve validation, risk analysis, and sensitivity analysis. Controllable variables lead to optimization, control, and what-if questions.

1. INTRODUCTION

Terms like parameters, scenarios, variables are often used in practice and in the literature without definition. In this contribution we shall define these terms and interpret their role in various types of models, concentrating on simulation and regression models. (These two model types are very popular in management practice; moreover, regression models may be used in the interpretation of simulation models; see Kleijnen (1981)). The user's view of the model leads to questions of validation, risk analysis, sensitivity analysis, optimization, etc. Table 1 summarizes our contribution; we shall refer to that table as we proceed.

2. TYPES OF VARIABLES

As the first column of Table 1 shows, we translate the simulation <u>model</u> into a simulation <u>program</u> (using a general programming language or a special simulation language). The simulation program has input and output.

The <u>output</u> of a simulation program may be called the simulation model's <u>response</u> (second column of Table 1). This output comprises one or more time series. We can characterize a time series through one or more measures, e.g., we may capture the waiting times of consecutive customers by their average or by their .90 quantile, i.e., we may summarize W_t with t = 1,2,...,T by \overline{W} and $W_{.90}$ where $W_{.90}$ is defined by P(W_t $\langle W_{.90} \rangle$ = 0.90. In this article we shall concentrate on a single response, i.e., a single time series characterized by a single measure,

TABLE 1

Computer	Simulation	Regression	User
program	model	model	view
program	model	model	VIEW
Output	Response	Dependent	Result
		variable	
		(y)	
Input	1. Parameter	Independent	l. Environmental
		variable	
	2. Variable	(x)	
	(i) Enumeration	(i) Continuous	(i) Validation
			(ii) Risk analysis
	(ii) Function	(ii) Discrete	2. Controllable
	(iii) Scenario	(iii) Binary	(i) Optimization
			(ii) Goal output
			(control)
			(iii) Satisficing
			(what-if)
	3. Behavioral		
	relationship		

Types of Variables

say, the average waiting time \overline{W} . In the terminology of regression analysis the response or output is called the <u>dependent</u> variable, usually denoted by the symbol y (third column). If we had multiple responses, we would speak of multivariate regression analysis.

The input of the simulation program can specify the simulation model's parameters, variables, and behavioral relationships. (Note that the input of a computer program might also be called the program's parameters, i.e., the program is a big subroutine or procedure that is called specifying the actual values of its parameters.) In a modeling context - to be distinguished from a programming context - we differentiate between variables and parameters. For instance, in a queuing model we may introduce a sequence of observed or actual service times s_1, s_2, \ldots . (We may use these actual values when validating the model.) Alternatively, we may sample the consecutive service times s1,s2,... from a statistical distribution (like the exponential distribution) with its "parameter" (say, λ); this distribution forms a submodel (for the service process) of the total queuing model. The difference between the variables and the parameters of a model is as follows: a variable is directly observable whereas a parameter requires statistical inference. Another difference is that a parameter remains constant during a simulation run; a variable may change during the run.

In the above terminology the number of service stations is a variable, not a parameter. And a <u>sequence</u> of actual service times is a sequence of variables. Actually we have several techniques for specifying such a time series:

(i) <u>Enumeration</u>: we list the individual values of the sequence. We use such enumeration when validating the simulation model. Note that the sequence may consist of a single value, e.g., the number of servers.

(ii) <u>Functional</u> specification: we specify a mathematical function like $x_t = a_1 + a_2 t$. In deterministic simulations we often specify a trend, a sinus, a ramp function, etc. In random simulations we specify the sequence of variables by their distribution function (e.g., the exponential distribution with parameter λ) plus the random number seed. The parameters (like a_1 , a_2 , λ) of the functional specification should be inferred from historical data.

(iii) <u>Scenarios</u>: this term we reserve for complicated, dynamic specifications. An example is: "a single server is available as long as individual queuing times do not exceed five minutes; a second server becomes available whenever that server has not been active during the last ten minutes and ..." A different scenario changes the values (five, ten) and possibly the rules ("... and more than one hour until closing time remains"). The word "scenario" is currently very popular and often used without definition. For a more general discussion of scenarios we refer to Becker (1981).

A <u>behavioral relationship</u> specifies the model's reaction to changes in its parameters and variables. Mathematically, a behavioral relationship is a function (such as y = 2x + 5) excluding tautologies, i.e., mathematical identities (such as $\overline{W} \equiv \sum_{i=1}^{n} W_i/n$). In our queuing example an interesting behavioral relationship is the priority rule or queuing discipline (first-in-first-out, shortest-jobs-first, etc.). A different priority rule may be evoked by calling a computer subroutine using different input values. For example, Hellerman and Conroy (1975,

p. 113) execute priority rules by finding the customer with the <u>minimum</u> value for the "service variable" SV; hence if the queuing discipline is first-come-first-served then SV equals arrival time AT; however, if small-jobs-first is the rule then SV equals service time ST. Consequently, we may specify the actual priority rule by a binary variable, say X and a programming instruction like "if X = 0 then SV = AT else SV = ST". (Obviously other programming styles are possible.) We shall return to this example when discussing binary variables in regression analysis.

So the input of the simulation program specifies the simulation model's parameters, variables, and behavioral relationships. In the terminology of regression analysis, these inputs are called the <u>indepen-</u> <u>dent</u> variables, usually denoted by x. If we have more than a single x then we speak of multiple regression analysis. How do the simulation model's parameters, variables and relationships correspond to the regression variables?

(i) Consider a simulation <u>parameter</u> (like the exponential distribution's parameter λ or the trend parameter a_2) which specifies a sequence of variables. This simulation parameter may correspond to a continuous regression variable, e.g., $x_1 = \lambda$. The independent variables x may also correspond to functions of the simulation parameters, e.g., $x_2 = \lambda^2$. (ii) A single <u>variable</u> like "number of servers" NS is handled in regression analysis exactly as parameters are handled. For instance, $x_1 = NS$ or $x_1 = (NS)^2$, etc. Discrete variables (like x = NS) and continuous variables (like x = λ) are treated identically in regression analysis. (iii) Differences among <u>scenarios</u> cannot be quantified so simply. Similar problems arise when we use different enumerations or behavioral relationships in the simulation model. These differences are qualitative

rather than quantitative. We can represent qualitative differences among simulation models by using a regression model with <u>binary</u> variables, i.e., x is zero or one: see the example in the preceding paragraph with the service variable SV. Note that sometimes binary variables are called dummy variables, but we reserve the term "dummy" for a variable that remains constant, i.e., in regression analysis the constant β_0 corresponds with $x_0 = 1$. Next we shall examine the differences between "qualitative" and "quantitative" in more detail.

3. MEASUREMENT SCALES AND REGRESSION

Oualitative phenomena are measured on a nominal scale whereas quantitative phenomena are measured on an interval, a ratio or an absolute scale. We consider these four scales in more detail, because their differences are important when using regression analysis (the literature gives more types of scales; Hauser and Shugan (1980), Sprent (1981)): (i) <u>Nominal</u> scale, for instance, machine type A, B or C; priority rule 1 (first-in-first-out) or rule 2 (last-in-first-out). In these examples the letters A, B, C and the numbers 1 and 2 are short-hand notations (mnemonics) used to distinguish priority rules; they imply no ranking. (ii) <u>Interval</u> scale: this scale does rank objects, but it has an arbitrary zero point so that an object with value 2x is "better" than an object with value x but it is not twice as good. Examples are: - Intelligence measured by the intelligence quotient (IQ): a person with

an IQ (according to a specific test) of 140 is not twice as smart as one with an IQ of 70.

- Temperature measured in Celsius (x^*) or Fahrenheit (x), related by the equation

$$x^* = (x - 32).(5/9)$$
(1)

Note that 20° C is not twice as warm as 10° C, which is clearly demonstrated when we choose a different scale such as Fahrenheit.

(iii) <u>Ratio</u> scale: this scale implies a ranking among objects; moreover it has a meaningful zero point such that 2x means "twice as much as x". Examples are length, measured in centimeters or inches (and the derived measures for surface and volume); angles measured in degrees or radians; richness measured in U.S. dollars or Dutch guilders. Different ratio scales are related by a linear transformation like eq. (1) but with a zero intercept, e.g., centimeters (x^{*}) and inches (x) are related by

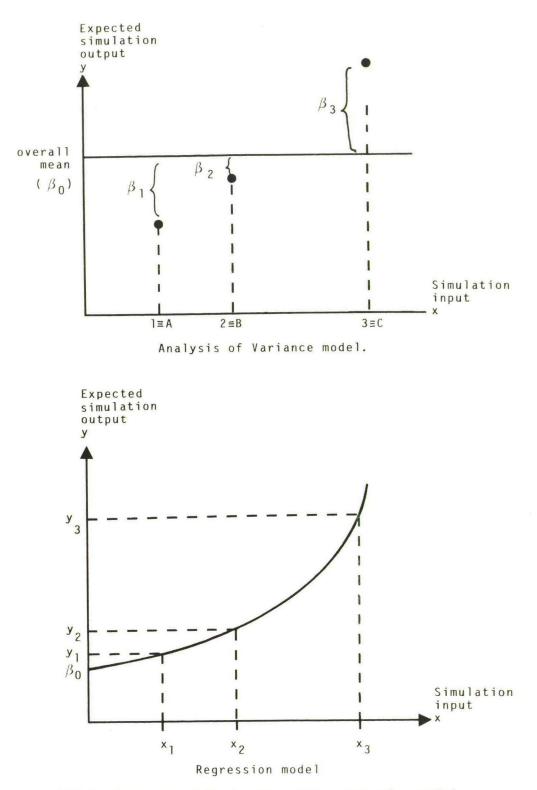
$$x^* = 2.56 x$$
 (2)

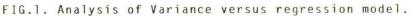
(iv) <u>Absolute</u> scale: no transformulation is applicable. Examples are provided by the counting of the number of servers, or the number of customer arrivals. Counting results in integer values: 0,1,2,3,... Note that counting processes may be the object of statistical laws like the binomial and the Poisson distributions.

As we acquire more operational knowledge about a problem, we proceed from a nominal to an interval and next to a ratio scale. In science we have acquired a good grip on certain topics such as measuring length and monetary richness, for which we have ratio scales (even temperature we can now measure on Kelvin's ratio scale). Other topics still have an arbitrary zero: intelligence, utility, etc. In mathematical statistics we may quantify the type of distribution through the parameter value of a family of distributions. For example, the exponential is a member of the Erlang family which is a member of the Gamma family.

A qualitative variable is measured on a nominal scale, whereas a quantitative variable is measured on one of the remaining three scales (interval, ratio, absolute scale). Regression analysis handles all scales in the same way, i.e., the regression model has independent variables x and some x may be binary, representing qualitative variables, and some other x may be discrete or continuous. However, in the interpretation of the regression results we have to be more careful: If we can measure a variable on a ratio scale then no interpretation problems arise, e.g., it does not matter whether we measure length in centimeters or inches. But, if we use an interval scale and there are interactions among variables, then we have to be more careful. Our practical advice is: measure the variable on the scale to which the user is accustomed. For instance, if the user measures temperature in Fahrenheit then the analyst should use that scale too; the regression coefficient β then represents the effect on the response when changing temperature by one degree Fahrenheit. In Appendix 1 we discuss standardization of variables in detail.

Interpolation (and extrapolation) make no sense for qualitative variables. A regression model which has only qualitative variables is known as <u>Analysis of Variance</u> or ANOVA; see FIG. 1. In ANOVA we test whether a factor has <u>any</u> effect at all; the effect at "value" i (with i = 1,2,3) of the factor is denoted by β_i in the figure (we can derive that $\Sigma\beta_i = 0$). In regression analysis, we are more ambitious: we quant-





ify <u>how much</u> the response reacts to changes in the factor; this quantification implies that we can test whether the factor has no effect: is the regression curve "flat" (zero regression parameters β except for the y-intercept β_0)? Note that if both quantitative and qualitative variables are present in the model then we speak of Analysis of Covariance (ANCOVA).

Consider an independent variable x_j which is quantitative (and assume that the regression curve is a straight line; for nonlinear models we refer to Appendix 1, eq. (1.7)). Then β_j measures the change of the expected output <u>per unit</u> change of x_j . The total change as x_j varies over its whole domain (L_j, U_j) equals the product β_j $(U_j - L_j)$; see FIG. 2. Consequently if the independent variables x_1 and x_2 have different ranges (R = U-L) then the total effect of x_1 may be larger than the total effect of x_2 even if $\beta_1 < \beta_2$; Also see Fiacco and Ghaemi (1982, pp. 17-19). Obviously if β is zero then the size of the range has no effect. Fortunately, significance tests can detect the unit effect β easier as the range of the (original) variable is larger: We can prove that the variance of the estimated effect decreases as the range increases, and consequently the significance test has more power. For qualitative variables β does not measure a "unit" effect.

4. USER VIEW: RISK AND SENSITIVITY ANALYSIS

The <u>user</u> of the simulation model (the manager, government agency, commanding officer) makes a different distinction among variables: environmental or exogenous variables versus controllable or instrumental variables; see Table 1 and FIG. 3.

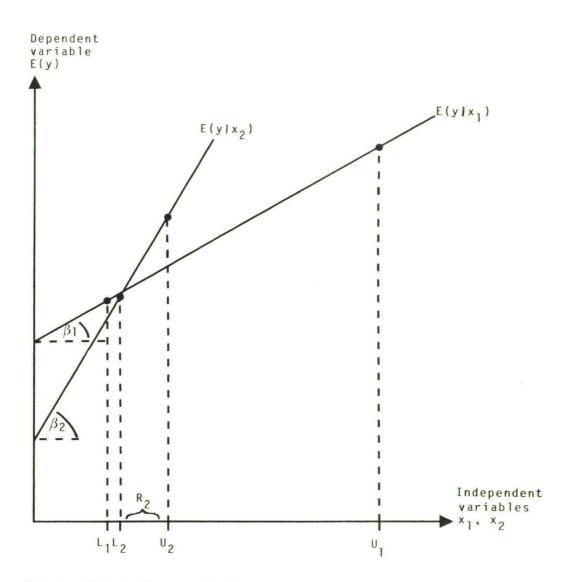


FIG.2. Effect of range R of independent variable

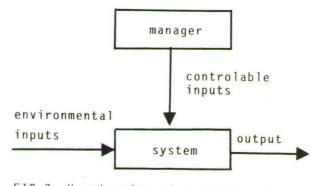
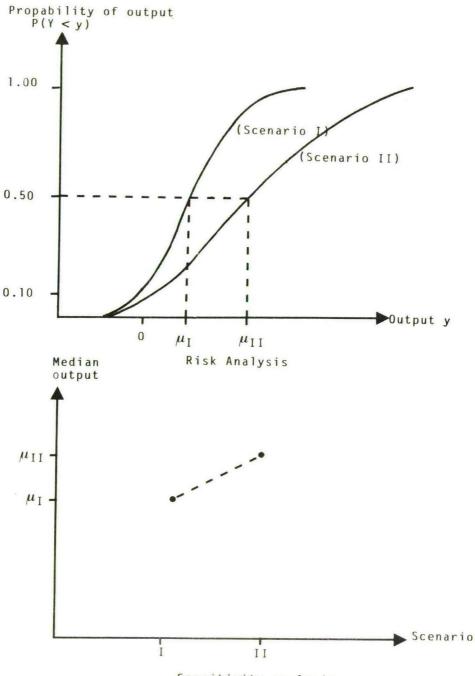


FIG.3. User's view of modeled system

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Environmental variables are not under the user's (immediate) control; an example is the arrival rate of customers (we ignore longrange effects via marketing, etc.). Therefore we must try to find out how sensitive the output is to the environmental variables. If that sensitivity is high then we may try to obtain information about the exact value of this input. Sometimes accurate information can indeed be obtained, e.g., more interarrival times may be collected by going back to historical data or by collecting more recent data. Anyhow, in so far as a model represents future behavior of the system, we need information on future input. If the environment shows little variation ("placid" environment) then we may analyse historical data and ignore the uncertainty of future input. If the output, however, is sensitive to the environmental input and information about that input is not accurate then the validity of te model is questionable. If the environmental input corresponds to a qualitative variable (e.g., type of scenario) then we may formulate several model variants; and if we cannot say which variant is valid then the user has to rely on his intuition when implementing recommendations based on different model variants. If the environmental input, however, represents a quantitative variable (such as an arrival rate) then we may specify a distribution of possible values for that variable based either on (objective) historical data or on (subjective) expert opinion. Next we can estimate the probability of a specific output by (Monte Carlo) sampling from the distribution of the input; so-called Risk Analysis. Examples of Risk Analysis, including case studies, can be found in Kleijnen (1980); also see Appendix 2.



Sensitivity analysis

FIG.4. Risk Analysis and sensitivity Analysis.

Note that we might subject Risk Analysis to sensitivity analysis. FIG. 4 illustrates that we can repeat the Risk Analysis exercise with different qualitative environmental inputs, say, different scenarios. The Risk Analysis output may be summarized by a single measure, e.g., the median (if the distribution is symmetric then the mean μ and the median $y_{.50}$ coincide; for simplicity's sake we denote the median by μ in FIG. 4). Other measures of interest may be the 0.10 quantile or the probability of negative output (see the point 0.10 on the vertical axis and the point 0 on the horizontal axis). In Risk Analysis we <u>sample</u> the input values whereas in sensitivity analysis we change the input systematically (one exception is sensitivity analysis based on random experimental designs).

5. USER VIEW: OPTIMIZATION AND WHAT-IF

The remaining elements of Table 1 refer to inputs which are under the user's control:

(i) Our most ambitious goal is to find the <u>optimal</u> solution, and a technique for maximalization of the output is Response Surface Methodo-logy; see Kleijnen (1985) and Myers (1971).

(ii) Sometimes the output level is prespecified, and our goal becomes to find a solution that yields this specified value: <u>control</u> problem. Instead of a trial-and-error approach to this control problem, we may follow a procedure based on regression modeling; see Appendix 3.

(iii) Simon (1960) emphasized that in practice users are not interested in the optimal solution and that they settle for an acceptable or "satisficing" solution. This attitude corresponds to the "what if" approach: make a change in the model (qualitative or quantitative change) and see what happens to the output (also see the Industrial or System Dynamics approach to socio-technical problems). It is ideal if our solution is robust, i.e., our advise to the user is not sensitive to the precise specification of our model.

6. SUMMARY

We distinguish output (response) and input of the system. The input of a simulation model are parameters, variables and behavioral relationships. In regression models the output is called the dependent variable; the inputs are the independent variables, some of which may be binary variables. The user's "model" distinguishes variables that are under his control or that are environmental. Environmental variables must be accurately specified to achieve model validity. Quantitative environmental variables (parameters) may be sampled: risk analysis. Control-lable variables may be optimized or they may be selected such that a specific output level is realized. In the what-if approach we determine what happens to the output if we change one or more inputs.

APPENDIX 1. CODING OF VARIABLES

Consider the regression model with main effects β_{j} and interactions β_{ji} :

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j \cdot x_j + \sum_{j=1}^{k} \beta_j j' \cdot x_j \cdot x_j + e \quad (1.1)$$

where the x are standardized variables, i.e., each x_j ranges between minus one and plus one with an average value of zero. We can standardize the original variables, say, z_j ranging between L_j and U_j , by the following linear transformation:

$$x_{j} = a_{j} + b_{j} \cdot z_{j} \text{ with } a_{j} = \frac{L_{j} + U_{j}}{L_{j} - U_{j}}$$

and
$$b_{j} = -2/(L_{j} - U_{j}) \qquad (1.2)$$

The eqs. (1.2) and (1.1) yield the regression model in the original variables z with regression parameters γ :

$$\mathbf{y} = \mathbf{\gamma}_{0} + \sum_{j} \mathbf{\gamma}_{j} \cdot \mathbf{z}_{j} + \sum_{j} \sum_{j} \mathbf{\gamma}_{jj} \cdot \mathbf{z}_{j} \cdot \mathbf{z}_{j} \cdot \mathbf{z}_{j}, + \mathbf{e}$$
(1.3)

where the following relations hold among the "standardized" effects β and the "original" effects $\gamma\colon$

$$Y_0 = \beta_0 + \sum_{j} a_j \cdot \beta_j + \sum_{j} \sum_{j} a_j \cdot a_j \cdot \beta_{jj}, \qquad (1.4)$$

$$\gamma_{j} = b_{j} \beta_{j} + b_{j} \beta_{j} \alpha_{j} \beta_{j} \beta_{j}$$

$$\gamma_{ij} = b_{j} \cdot b_{j} \cdot \beta_{ij}$$
(1.6)

Consequently, if there are no interactions $(\gamma_{jj}, = \beta_{jj}, = 0;$ see eq. 1.6) then zero main effects of the standardized variables $(\beta_j = 0)$ imply zero main effects of the original variables; see eq. (1.5). However, if there are interactions then zero main effects β_j do <u>not</u> imply zero main effects γ_j . We can compute the marginal responses $\partial y/\partial z_j$ from the regression model for the standardized variables or from the regression model in the original variables. For instance, $\partial y/\partial z_j$ if z_j , = 0 with j' \neq j is computed from eq. (1.3) as γ_j ; from eqs. (1.1) and (1.2) it follows that for z_j , = 0 or x_j , = a_j .

$$\frac{\partial y}{\partial z_{j}} = \frac{\partial y}{\partial x_{j}} \cdot \frac{\partial x_{j}}{\partial z_{j}} = (\beta_{j} + \sum_{j'} \beta_{jj'} \cdot a_{j'}) \cdot b_{j} = \gamma_{j}$$
(1.7)

More about coding can be found in Mendenhall (1968, pp. 221-229, 251-257) and Mihram (1972, pp. 359-360).

APPENDIX 2. RISK ANALYSIS ON REGRESSION MODELS

Consider the following simplistic model (related but more realistic models are used in, e.g., econometrics):

$$y_t = \beta_0 + \beta_1 \cdot x_t + e_t$$
 (2.1)

where $e_t \sim \text{NID}(0, \sigma^2)$. Obviously, given this specification of the model, the unknown parameters are the β 's and σ . These unknown parameters can be estimated through the regression analysis of, say, T historical data points. The standard errors - or more generally the covariance matrix - of the $\hat{\beta}$'s are given by $(X'X)^{-1}\sigma^2$. It can further be proved - see, e.g., Johnston (1972, p. 26) - that $\hat{\sigma}^2$ has a χ^2 - distribution with T-2 degrees of freedom and that $\hat{\sigma}^2$ is independent of the β estimators.

Suppose that we computed the estimated parameters $\hat{\beta}$ and $\hat{\sigma}^2$ for the above regression model, using (historical) data from the (sampling) period t = 1,...,T. And next we wish to use the estimated model for "<u>forecasting</u>". Several alternatives seem reasonable: <u>Case 1(a)</u>: Predict <u>the</u> most likely value for the <u>next</u> period t = T+1, given the independent variable x_{T+1} . An estimator is:

$$\hat{y}_{T+1} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+1}$$
 (2.2)

This value is also an unbiased estimator of the <u>expected</u> value for the period T+1:

$$E(\hat{y}_{T+1}) = E(\hat{\beta}_0) + E(\hat{\beta}_1) \cdot x_{T+1} = \beta_0 + \beta_1 \cdot x_{T+1} = E(y_{T+1})$$
 (2.3)

<u>Case 1(b)</u>: We can derive the <u>probability</u> of values different from the most likely or expected value as follows: The estimated analogue of eq. (2.1) is

$$\tilde{y}_{T+1} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+1} + \hat{e}_{T+1}$$
 (2.4)

where $\hat{e}_{T+1} \sim N(0, \sigma^2)$. Since \tilde{y}_{T+1} is a linear combination of the normally distributed variables $\hat{\beta}_0$, $\hat{\beta}_1$ and \hat{e}_{T+1} we know that \tilde{y}_{T+1} is normally distributed. Its mean was given by eq. (2.3); its variance is

$$var(\tilde{y}_{T+1}) = var(\hat{\beta}_{0}) + (x_{T+1})^{2} \cdot var(\hat{\beta}_{1}) + + 2x_{T+1} \cdot cov(\hat{\beta}_{0}, \hat{\beta}_{1}) + var(\hat{e}_{T+1})$$
(2.5)

Note that $cov(\hat{e}_{T+1}, \hat{\beta}) = 0$ because $\hat{\beta}$ depends on (y_1, \dots, y_T) and not on y_{T+1} , and the error terms are serially independent. In the first paragraph of this appendix we referred to estimators for the terms in eq. (2.5). Finally, using the table for the standard normal variable N(0,1), we can compute the probability of values \tilde{y}_{T+1} different from the most likely value \hat{y}_{T+1} .

<u>Case 2(a)</u>: Predict <u>several</u> periods ahead, e.g., predict the response for T+1 and T+2. Now the example of eq. (2.1) is too simple to illustrate what is at stake. Therefore we introduce a slightly more complicated example, including a lagged dependent variable: eq. (2.1) is replaced by

$$y_t = \beta_0 + \beta_1 \cdot x_t + \beta_2 \cdot y_{t-1} + e_t$$
 (2.6)

Consequently the most likely value or the expected value for period T+1 is no longer estimated by eq. (2.2) but by the unbiased estimator

$$\hat{y}_{T+1} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+1} + \hat{\beta}_2 \cdot y_T$$
 (2.7)

where y_{T} is an observed (sample) value. However, when we extrapolate for more than one period ahead, we obtain:

$$\hat{y}_{T+2} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+2} + \hat{\beta}_2 \cdot \hat{y}_{T+1}$$
 (2.8)

where the last term uses the estimator given by eq. (2.7). Unfortunately eq. (2.8) is <u>biased</u>: for the last term of eq. (2.8) the following inequality holds because the random variable \hat{y}_{T+1} depends on the random variable $\hat{\beta}_2$:

$$E(\hat{\beta}_2, \hat{y}_{T+1}) \neq E(\hat{\beta}_2) \cdot E(\hat{y}_{T+1}) = \beta_2 \cdot E(y_{T+1})$$
 (2.9)

Therefore we may resort to simulation: for t > T we sample \hat{e}_t from $(0, \sigma^2)$; this \hat{e}_t yields \tilde{y}_t (see eq. 2.4); etc.

<u>Case 2(b)</u>: It is straightforward to compute the <u>probability</u> of values different from the most likely value or the expected value in period T+1, but it is complicated to compute this probability for period T+2:

$$\tilde{y}_{T+1} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+1} + \hat{\beta}_2 \cdot y_T + \hat{e}_{T+1}$$
 (2.10)

and

$$\tilde{y}_{T+2} = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_{T+2} + \hat{\beta}_2 \cdot \tilde{y}_{T+1} + \hat{e}_{T+2}$$
 (2.11)

Again simulation provides the answer.

We emphasize that some values of y_{T+2} are "impossible", given that y_{T+1} has a particular value (under the normality assumption theoretically all values are possible; however the probability of "extreme" values is virtually zero). So some time paths are virtually impossible.

Summarizing, in cases l(a) and 2(a) we estimated the expected value one period ahead and two periods ahead respectively. If we forecast several periods ahead, we may use simulation. In cases l(b) and 2(b) we were interested in the probability of deviations from these values. The latter probabilistic element entered through the random noise e, estimated by \hat{e} .

A different chance element enters our analysis, if we realize that the model itself may be incorrect! More specifically, even if we assume that we specified the correct <u>form</u> (i.e., a linear model) then we may still use the wrong <u>parameter</u> values: the estimators $\hat{\beta}_0$ and $\hat{\beta}_1$ are not precisely equal to β_0 and β_1 , and $\hat{\sigma}^2$ is not exactly equal to σ^2 . Therefore we may apply <u>risk analysis</u>: we can sample $\hat{\beta}_0$ and $\hat{\beta}_1$ in the eqs. (2.2) through (2.11) from a bivariate normal distribution (with mean and covariance matrix given by the standard regression analysis of the historical time series) and we can sample $\hat{\sigma}^2$ from the χ^2_{T-2} distribution; see the first paragraph of this appendix.

We can combine each of the (say n_1) sampled triplets $(\hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)$ of the risk analysis with each of the (say n_2) simulated time paths obtained by sampling the disturbances $(\hat{e}_{T+1}, \hat{e}_{T+2})$, and this combination results in an $n_1 \times n_2$ table. From the n_2 observations per row we might estimate the conditional probabilities $P(y_{T+2}, \hat{\beta}_0, \hat{\beta}_1, \hat{\sigma}^2)$. However, the purpose of the risk analysis is to estimate the unconditional probabilities $P(y_{T+2})$ which incorporates noise around the expected value plus noise in the estimation of the model's parameters. From these unconditional probabilities we can compute the mean and median response, the probability of negative responses, etc. Note that it would be incorrect to use the following risk analysis procedure (which at first sight might look reasonable): (i) Sample $\hat{\beta}_0$ and $\hat{\beta}_1$.

(ii) Comupute the corresponding historical values

$$\hat{y}_t = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_t$$
 (t = 1,...,T) (2.12)

(iii) Compute the corresponding historical residuals

$$u_t = y_t - y_t$$
 (t = 1,...,T) (2.13)

These residuals no longer satisfy the Least Squares properties such as $\Sigma u_t = 0.$ (iv) Compute the corresponding $\hat{\sigma}^2$:

$$\hat{\sigma}^2 = \Sigma u_{+} / (T-2)$$
 (2.14)

This estimator is no longer an optimal estimator of σ^2 ; see the comment on step (iii).

APPENDIX 3. INVERSE REGRESSION IN CONTROL PROBLEMS

In the control problem we have a target value for the response, and we wish to estimate the values for the instrumental variables, given specific values for the environmental variables. The simplest solution is to proceed "as usual", i.e., estimate E(y) as a function of the k independent variables (k = $k_1 + k_2$ where k_1 denotes the number of instrumental variables and k_2 is the number of environmental variables; the latter

variables are shown in parentheses):

$$E(y) = \hat{\beta}_0 + \hat{\beta}_1 \cdot x_1 + \dots + \hat{\beta}_{k_1} \cdot x_{k_1} (+ \dots + \hat{\beta}_k \cdot x_k) \quad (3.1)$$

The simplest situation arises if we have a single controllable variable $(k_1 = 1)$. Then we can estimate the required value of x_1 , say x_1^* , from eq. (3.2) where y_c denotes the goal value:

$$\mathbf{x}_{1}^{*} = \frac{1}{\hat{\beta}_{1}} \left\{ \mathbf{y}_{G} - \hat{\beta}_{0} - (\hat{\beta}_{2} \cdot \mathbf{x}_{2} + \dots + \hat{\beta}_{k} \cdot \mathbf{x}_{k}) \right\}$$
(3.2)

However, there is an alternative estimator: We can regress x_1 on y (and on the prespecified values of the k_2 environmental variables where $k_2 \ge 0$):

$$x_1 = \gamma_0 + \gamma_1 \cdot y(+ \gamma_2 \cdot x_2 + \dots + \gamma_{k-1} \cdot x_{k-1}) + e$$
 (3.3)

A second estimator, say $x_1^{\star\star}$, results if we use the estimators γ and substitute y_G for y. Which estimator is best, is not clear, even in the simplest situations ($k_2 = 0$; $k_2 = 1$; Classical Assumptions for e); see Turiel et al. (1982) for a recent survey of the various statistical problems of "inverse" regression.

In simulation the situation is more complicated. The response is probably sensitive to several environmental variables $(k_2 > 1)$ and there are several controllable variables $(k_1 > 1)$. If $k_1 > 1$ then the second estimator x^{**} results in a system of simultaneous equations (see the third term in the following equations):

$$x_{1} = \gamma_{0} + \gamma_{1} \cdot y + \gamma_{2} \cdot x_{2} (+ \dots + \gamma_{k-1} \cdot x_{k-1}) + e_{1} \quad (3.4)$$

$$\mathbf{x}_{2} = \delta_{0} + \delta_{1} \cdot \mathbf{y} + \delta_{2} \cdot \mathbf{x}_{1} (+ \dots + \delta_{k-1} \cdot \mathbf{x}_{k-1}) + \mathbf{e}_{2}$$
(3.5)

The statistical problems of simultaneous regression equations are discussed in econometric handbooks. Fortunately, we can take advantage of the peculiarities of simulation, i.e., after we have used the regression metamodel to estimate the required value (or values) of the instrumental variable (or variables), we can check this solution by performing a simulation run with the indicated values for the instrumental variables and verifying whether the resulting output does not deviate significantly from the target value.

One more approach we would suggest is to transform the control problem into an optimization problem, i.e., select the control variables such that the deviation between the target value and the realized value of the dependent variable y is minimial. Such minimization problems can be approached through Response Surface Methodology.

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